## (12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

## (19) World Intellectual Property Organization International Bureau





# (43) International Publication Date 27 November 2003 (27.11.2003)

## **PCT**

# (10) International Publication Number WO 03/096984 A2

(51) International Patent Classification7:

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(21) International Application Number: PCT/US03/15506

(22) International Filing Date: 14 May 2003 (14.05.2003)

(25) Filing Language:

English

A61K

(26) Publication Language:

English

(30) Priority Data:

 60/380,761
 14 May 2002 (14.05.2002)
 US

 60/392,782
 28 June 2002 (28.06.2002)
 US

 60/422,933
 31 October 2002 (31.10.2002)
 US

 60/428,033
 20 November 2002 (20.11.2002)
 US

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- (81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.
- (84) Designated States (regional): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

#### Published:

 without international search report and to be republished upon receipt of that report

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

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(54) Title: DRUG THERAPY FOR CELIAC SPRUE

(57) Abstract: Celiac Sprue and/or dermatitis herpetiformis are treated by interfering with HLA binding of immunogenic gluten peptides. The antigenicity of gluten oligopeptides and the ill effects caused by an immune response thereto are decreased by administration of an HLA-binding peptide inhibitor. Such inhibitors are analogs of immunogenic gluten peptides and (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific T cells.



## DRUG THERAPY FOR CELIAC SPRUE

#### **CROSS-REFERENCE TO RELATED APPLICATIONS**

This application claims priority to U.S. Provisional Application 60/380,761 filed May 14, 2002; to U.S. Provisional Application 60/392,782 filed June 28, 2002; and to U.S. Provisional application no. 60/422,933, filed October 31, 2002, and to U.S. Provisional Application 60/428,033, filed November 20, 2002, each of which are herein specifically incorporated by reference.

### BACKGROUND OF THE INVENTION

In 1953, it was first recognized that ingestion of gluten, a common dietary protein present in wheat, barley and rye causes a disease called Celiac Sprue in sensitive individuals. Gluten is a complex mixture of glutamine- and proline-rich gliadin and glutenin molecules and is thought to be responsible for induction of Celiac Sprue. Ingestion of such proteins by sensitive individuals produces flattening of the normally luxurious, rug-like, epithelial lining of the small intestine known to be responsible for efficient and extensive terminal digestion of peptides and other nutrients. Other clinical symptoms of Celiac Sprue include fatigue, chronic diarrhea, malabsorption of nutrients, weight loss, abdominal distension, anemia, as well as an enhanced risk for the development of osteoporosis and intestinal malignancies such as lymphoma and carcinoma. The disease has an incidence of approximately 1 in 200 in European populations and is believed to be significantly under diagnosed in other populations.

A related disease is dermatitis herpetiformis, which is a chronic eruption of the skin characterized by clusters of intensely pruritic vesicles, papules, and urticaria-like lesions. IgA deposits occur in almost all normal-appearing and perilesional skin. Asymptomatic gluten-sensitive enteropathy is found in 75 to 90% of patients and in some of their relatives. Onset is usually gradual. Itching and burning are severe, and scratching often obscures the primary lesions with eczematization of nearby skin, leading to an erroneous diagnosis of eczema. Strict adherence to a gluten-free diet for prolonged periods may control the disease in some patients, obviating or reducing the requirement for drug therapy. Dapsone, sulfapyridine, and colchicines are sometimes prescribed for relief of itching.

[03]

Celiac Sprue (CS) is generally considered to be an autoimmune disease and the antibodies found in the serum of the patients support the theory that the disease is immunological in nature. Antibodies to tissue transglutaminase (TG2, tTGase or tTG) and gliadin appear in almost 100% of the patients with active CS, and the presence of such antibodies, particularly of the IgA class, has been used in diagnosis of the disease.

[DQ(a1\*03, b1\*0302)] molecules. It is believed that intestinal damage is caused by interactions between specific gliadin oligopeptides and the HLA-DQ2 or DQ8 antigen, which in turn induce proliferation of T lymphocytes in the sub-epithelial layers. T helper 1 cells and cytokines apparently play a major role in a local inflammatory process leading to villous atrophy of the small intestine.

At the present time, there is no good therapy for the disease, except to avoid completely all foods containing gluten. Although gluten withdrawal has transformed the prognosis for children and substantially improved it for adults, some people still die of the disease, mainly adults who had severe disease at the outset. A leading cause of death is lymphoreticular disease, especially intestinal lymphoma. It is not known whether a glutenfree diet diminishes this risk. Apparent clinical remission is often associated with histologic relapse that is detected only by review biopsies or by increased titers of antibodies to tTGase (also called EMA antibodies).

Gluten is so widely used, for example, in commercial soups, sauces, ice creams, hot dogs, and other foodstuffs, that patients need detailed lists of foodstuffs to avoid and expert advice from a dietitian familiar with celiac disease. Ingesting even small amounts of gluten may prevent remission or induce relapse. Supplementary vitamins, minerals, and hematinics may also be required, depending on deficiency. A few patients respond poorly or not at all to gluten withdrawal, either because the diagnosis is incorrect or because the disease is refractory. In the latter case, oral corticosteroids (e.g., prednisone 10 to 20 mg bid) may induce response.

In view of the serious and widespread nature of Celiac Sprue and the difficulty of removing gluten from the diet, better methods of treatment are of great interest. In particular, there is a need for treatment methods that allow the Celiac Sprue individual to eat gluten-containing foodstuffs without ill effect or at least to tolerate such foodstuffs in small or moderate quantities without inducing relapse. The present invention meets this need for better therapies for Celiac Sprue.

## SUMMARY OF THE INVENTION

[09] In one aspect, the present invention provides methods for treating Celiac Sprue and/or dermatitis herpetiformis and the symptoms thereof by administration of an HLA-binding peptide inhibitor to the patient. In one embodiment, the HLA-binding peptide inhibitor employed in the method is an analog of an immunogenic gluten peptide, where an immunogenic gluten peptide is altered by the replacement of one or more amino acids, where the replacement may be another naturally occurring amino acid, non-naturally occurring amino acids, modified amino acids, amino acid mimetics, and the like. Analogs of

immunogenic gluten peptides that (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells, are useful agents to treat Celiac Sprue.

[10] In another aspect, the present invention provides novel HLA-binding peptide inhibitors and methods for treating Celiac Sprue and/or dermatitis herpetiformis by administering those compounds.

In another aspect, the invention provides pharmaceutical formulations comprising an HLA-binding peptide inhibitor and a pharmaceutically acceptable carrier. In one embodiment, such formulations comprise an enteric coating that allows delivery of the active agent to the intestine, and the agents are stabilized to resist digestion or acid-catalyzed modification in acidic stomach conditions. In another embodiment, the formulation also comprises one or more glutenases, as described in U.S. Provisional Application 60/392,782 filed June 28, 2002; and U.S. Provisional Application 60/428,033, filed November 20, 2002, both of which are incorporated herein by reference. The invention also provides methods for the administration of enteric formulations of one or more HLA-binding peptide inhibitors to treat Celiac Sprue.

[12] In another aspect, the invention provides methods for screening candidate compounds to determine their suitability for use in the subject methods, by assessing the ability of a candidate agent for its ability to bind to HLA molecules, and/or to inhibit the activity of T cells reactive against gluten antigens.

[13]

Methods and compositions are provided for modeling the structure of a soluble (extracellular) domain of human HLA-DQ2 bound to an immunodominant gluten epitope, and for identifying molecules that will compete with the gluten peptide for MHC binding. In one embodiment, the methods of the invention utilize structural modeling, and the identification and design of molecules having a particular structure. The structural data provided herein is used for the rational design of drugs that affect immune system activation in Celiac Sprue and/or dermatitis herpetiformis. Analysis of the crystal structure in conjunction with sequence data identifies residues in the immunogenic gluten peptide that are important for interaction with the MHC molecule, and those that are accessible for interaction with the T cell antigen receptor. This information provides a basis for rational drug design.

[14] These and other aspects and embodiments of the invention and methods for making and using the invention are described in more detail in the description of the drawings and the invention, the examples, the claims, and the drawings that follow.

## **DETAILED DESCRIPTION OF THE EMBODIMENTS**

Celiac Sprue and/or dermatitis herpetiformis are treated by interfering with HLA binding of immunogenic gluten peptides. Therapeutic benefit can be enhanced in some individuals by increasing the digestion of gluten oligopeptides, whether by pretreatment of foodstuffs to be ingested or by administration of an enzyme capable of digesting the gluten oligopeptides, together with administration of an HLA-binding peptide inhibitor. Gluten oligopeptides are highly resistant to cleavage by gastric and pancreatic peptidases such as pepsin, trypsin, chymotrypsin, and the like, and their prolonged presence in the digestive tract can induce an autoimmune response. The antigenicity of gluten oligopeptides and the ill effects caused by an immune response thereto can be decreased by administration of an HLA-binding peptide inhibitor. Such inhibitors are analogs of immunogenic gluten peptides and (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells.

Methods and compositions are provided for the administration of one or more HLA-binding peptide inhibitors to a patient suffering from Celiac Sprue and/or dermatitis herpetiformis. In some embodiments and for some individuals, the methods of the invention remove the requirement that abstention from ingestion of glutens be maintained to keep the disease in remission. The compositions of the invention include formulations of tTGase inhibitors that comprise an enteric coating that allows delivery of the agents to the intestine in an active form; the agents are stabilized to resist digestion or alternative chemical transformations in acidic stomach conditions. In another embodiment, food is pretreated or combined with glutenase, or a glutenase is co-administered (whether in time or in a formulation of the invention) with an HLA-binding peptide inhibitor of the invention.

[17]

Thus, as used herein, the term "treating" is used to refer to both prevention of disease, and treatment of a pre-existing condition. The treatment of ongoing disease, to stabilize or improve the clinical symptoms of the patient, is a particularly important benefit provided by the present invention. Such treatment is desirably performed prior to loss of function in the affected tissues; consequently, the prophylactic therapeutic benefits provided by the invention are also important. Evidence of therapeutic effect may be any diminution in the severity of disease, particularly diminution of the severity of such symptoms as fatigue, chronic diarrhea, malabsorption of nutrients, weight loss, abdominal distension, and anemia. Other disease indicia include the presence of antibodies specific for glutens, antibodies specific for tissue transglutaminase, the presence of pro-inflammatory T cells and cytokines, and degradation of the villus structure of the small intestine. Application of the methods and compositions of the invention can result in the improvement of any and all of these disease indicia of Celiac Sprue.

Patients that can benefit from the present invention include both adults and children. Children in particular benefit from prophylactic treatment, as prevention of early exposure to toxic gluten peptides can prevent development of the disease into its more severe forms. Children suitable for prophylaxis in accordance with the methods of the invention can be identified by genetic testing for predisposition, e.g. by HLA typing; by family history, and by other methods known in the art. As is known in the art for other medications, and in accordance with the teachings herein, dosages of the HLA-binding peptide inhibitors of the invention can be adjusted for pediatric use.

Because most proteases and peptidases are unable to hydrolyze the amide bonds of proline residues, the abundance of proline residues in gliadins and related proteins from wheat, rye and barley can constitute a major digestive obstacle for the enzymes involved. This leads to an increased concentration of relatively stable gluten derived oligopeptides in the gut. These stable gluten derived oligopeptides, called "immunogenic oligopeptides" herein, bind to MHC molecules, including HLA HLA-DQ2 or DQ8 molecules, to stimulate an immune response that results in the autoimmune disease aspects of Celiac Sprue. In some cases the enzyme tissue transglutaminase selectively deamidates certain glutamine residues in these peptides, thereby enhancing their potency for the DQ2 ligand binding pocket.

[20] HLA-binding peptide inhibitors of the present invention are analogs of immunogenic gluten oligopeptides that (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells. The inhibitor may comprise oligomers of analogs. Multivalent gluten derived epitopes have markedly enhanced immunogenicity. Consequently, multivalent oligopeptides analogs can also be expected to have increased potency for MHC molecules. In addition, these longer peptides can be more resistant toward intestinal brush border proteolysis.

[21]

An immunogenic gluten oligopeptide analog is an analog of a peptide that comprises at least about 8 residues, and may comprise at least about 10 residues; at least about 11 residues, at least about 12 residues, at least about 13 residues, at least about 14 residues, or more, where the term "residue" refers to naturally occurring amino acids, non-naturally occurring amino acids, and amino acid mimetics or derivatives; and where the gluten peptide is altered by the replacement of one or more amino acids. The replacement may be another naturally occurring amino acid, non-naturally occurring amino acids, modified amino acids, amino acid mimetics, and the like; and may further be derivitized to further reduce the affinity of these ligands for disease-specific T cell receptors. The sequence of immunogenic gluten oligopeptides can be determined by one of skill in the art. Immunogenic gliadin oligopeptides are peptides derived during normal human digestion of gliadins and related storage proteins as described above, from dietary cereals, e.g. wheat, rye, barley, and the

like. Such oligopeptides act as antigens for T cells in Celiac Sprue. For binding to Class II MHC proteins, immunogenic peptides are usually from about 8 to 20 amino acids in length, more usually from about 10 to 18 amino acids. Such peptides may include PXP motifs, such as the motif PQPQLP. Determination of whether an oligopeptide is immunogenic for a particular patient is readily determined by standard T cell activation and other assays known to those of skill in the art.

Among gluten proteins with potential harmful effect to Celiac Sprue patients are [22] included the storage proteins of wheat, species of which include Triticum aestivum; Triticum aethiopicum; Triticum baeoticum; Triticum militinae; Triticum monococcum; Triticum sinskajae; Triticum timopheevii; Triticum turgidum; Triticum urartu, Triticum vavilovii; Triticum zhukovskyi; etc. A review of the genes encoding wheat storage proteins may be found in Colot (1990) Genet Eng (N Y) 12:225-41. Gliadin is the alcohol-soluble protein fraction of wheat gluten. Gliadins are typically rich in glutamine and proline, particularly in the N-terminal part. For example, the first 100 amino acids of  $\alpha$ - and  $\gamma$ -gliadins contain ~35% and ~20% of glutamine and proline residues, respectively. Many wheat gliadins have been characterized, and as there are many strains of wheat and other cereals, it is anticipated that many more sequences will be identified using routine methods of molecular biology. Examples of gliadin sequences include but are not limited to wheat alpha gliadin sequences, for example as provided in Genbank, accession numbers AJ133612; AJ133611; AJ133610; AJ133609; AJ133608; AJ133607; AJ133606; AJ133605; AJ133604; AJ133603; AJ133602; D84341.1; U51307; U51306; U51304; U51303; U50984; and U08287. A sequence of wheat omega gliadin is set forth in Genbank accession number AF280605.

Among the immunogenic gluten oligopeptides that may be modified to generate an HLA-binding peptide inhibitor are included the peptide sequence QLQPFPQPELPYP; the sequence PQPELPY; the sequence PFPQPELPYP, PQPELPYPQPQLP, PQQSFPEQQPP, VQGQGIIQPEQPAQ, FPEQPQQPYPQQP, FPQQPEQPYPQQP, FSQPEQEFPQPQ and longer peptides containing such sequences or multiple copies of such sequences. Gliadins, secalins and hordeins contain several PQPQLPY sequences or sequences similar thereto rich in Pro-Gln residues that are high-affinity substrates for tTGase. The tTGase catalyzed deamidation of such sequences increases their affinity for HLA-DQ2, the class II MHC allele present in >90% Celiac Sprue patients. Presentation of these deamidated sequences by DQ2 positive antigen presenting cells effectively stimulates proliferation of gliadin-specific T cells from intestinal biopsies of most Celiac Sprue patients, providing evidence for the proposed mechanism of disease progression in Celiac Sprue.

[24] Analog oligopeptides of the invention comprise at least one difference in amino acid sequence from a native gluten peptide, by the replacement of an amino acid with a different

amino acid; a non-naturally occurring amino acid, a peptidomimetics, substituted amino acid, and the like. An L-amino acid from the native peptide may be altered to any other one of the 20 L-amino acids commonly found in proteins, any one of the corresponding D-amino acids, rare amino acids, such as 4-hydroxyproline, and hydroxylysine, or a non-protein amino acid, such as  $\beta$ -alanine, ornithine and homoserine. Also included with the scope of the present invention are amino acids that have been altered by chemical means such as methylation (e.g.,  $\alpha$ -methylvaline), deamidation, amidation of the C-terminal amino acid by an alkylamine such as ethylamine, ethanolamine, and ethylene diamine, and acylation or methylation of an amino acid side chain function (e.g., acylation of the epsilon amino group of lysine), deimination of arginine to citrulline, isoaspartylation, or phosphorylation on serine, threonine, tyrosine or histidine residues. Importantly, each of these altered amino acids provide a functional handle, e.g. amine, alcohol, aryl halide, and the like, which can be regioselectively derivatized to further reduce the affinity of these ligands for disease-specific T cell receptors. Peptide analogs may be further derivatized with substitutions, including, without limitation, ethers, amines, esters, amides, carbonates, carbamates, carbazates, ureas and C-C coupled derivatives. Other examples include oxidation of alcohols to ketones, followed by further modifications of the resulting carbonyl group, e.g. via preparation of oximes) or the carbon atom adjacent to the ketone. Such derivatives are encompassed by the term "analog".

[25] The proteolytic stability of gluten oligopeptides can be attributed, at least in part, to the presence of PXP motifs, which are resistant to enzymatic degradation. Preferred analogs of immunogenic gluten oligopeptides will comprise one or more proline residues, and may comprise one or more PXP motifs.

An immunogenic gluten peptide of particular interest is the 33-mer LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQPPP, which is described in detail in International Patent Application US03/04743, herein specifically incorporated by reference. This peptide is both immunogenic and highly stable to proteases. T cell epitopes present in the 33-mer peptide include, *inter alia*, PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PQPELPYPQ; PYPQPELPY and PYPQPQLPY. In one embodiment of the invention, the immunogenic gluten oligopeptide analog is an analog of a peptide that comprises at least one T cell epitope selected from the group consisting of PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PQPELPYPQ; PYPQPELPY and PYPQPQLPY.

The structure of an immunogenic gluten oligopeptide bound to a presenting molecule, e.g. HLA-DQ2; HLA-DQ8; etc. can be determined, e.g. by crystallography, NMR, etc., and used to identify residues in a peptide that are involved in the binding to the MHC molecule, and that are involved in the binding to a T cell antigen receptor. Residues identified as accessible for interacting with the T cell receptor may be modified to decrease

the interaction, e.g. by increasing steric hindrance, altering hydrophilicity or hydrophobicity, etc. Residues identified as involved in interaction with the binding cleft of an MHC molecule may be modified to increase the interaction, e.g. by incorporating amino acids known to interact strongly with the binding cleft.

One inhibitor of interest is an oligopeptide or peptidomimetic that comprises the sequence PXPQPELPY, where X is Gly, Ala, Tyr, Trp, Arg, Lys, p-iodo-Phe, 3-iodo-Tyr, p-amino-Phe, 3-amino-Tyr, hydroxylysine, ornithine, Asp, Glu, or any residue that is substantially bulkier or hydrophilic than Phe. Examples of suitable modifications include ethers, amines, esters, amides, carbonates, carbamates, carbazates, ureas and C-C coupled derivatives. Other examples include oxidation of alcohols to ketones, followed by further modifications of the resulting carbonyl group (e.g. via preparation of oximes) or the carbon atom adjacent to the ketone. The peptide may comprise modifications that increase binding potency to an MHC molecule, by varying residues that facilitate peptide docking into the binding cleft. Examples of such residues include Gln-4, Glu-6, Leu-7, and Tyr-9 (numbering based on the epitope PFPQPELPY). Each of these residues interacts closely with several residues in the DQ2 binding pocket. By using structure-based molecular design methods, these interactions can be optimized.

[29] Another inhibitor of interest is a oligopeptide or peptidomimetic that comprises the sequence PFPQX<sub>1</sub>ELX<sub>2</sub>Y, where X<sub>1</sub> and X<sub>2</sub> are independently selected from 4-hydroxy-Pro (either isomer at C-4), 4-amino-Pro (either isomer atC-4), or 3-hydroxy-Pro (either isomer atC-3), and proline, with the proviso that at least one of X<sub>1</sub> and X<sub>2</sub> is a residue other than proline.

Peptides and peptide analogs may be synthesized by standard chemistry techniques, including synthesis by automated procedure. In general, peptide analogs are prepared by solid-phase peptide synthesis methodology which involves coupling each protected amino acid residue to a resin support, preferably a 4-methylbenzhydrylamine resin, by activation with dicyclohexylcarbodiimide to yield a peptide with a C-terminal amide. Alternatively, a chloromethyl resin (Merrifield resin) may be used to yield a peptide with a free carboxylic acid at the C-terminus. After the last residue has been attached, the protected peptide-resin is treated with hydrogen fluoride to cleave the peptide from the resin, as well as deprotect the side chain functional groups. Crude product can be further purified by gel filtration, HPLC, partition chromatography, or ion-exchange chromatography.

[31] The present invention provides crystals and structures of HLA-DQ2 bound to antigen, where the antigen is an immunogenic gluten peptide QLQPFPQPELPYP, which may be referred to for brevity as an "HLA-DQ2/peptide complex". The structures and structural coordinates are useful in structural homology deduction, and in developing and

screening agents that affect the gluten antigen presentation and immunogenicity. The structure information may be provided in a computer readable form, *e.g.* as a database of atomic coordinates, or as a three-dimensional model. The structures are useful, for example, in modeling interactions of the HLA molecule with the antigen, effect of inhibitors, *etc.* The structures are also used to identify molecules that bind to or otherwise interact with structural elements. One aspect of the present invention provides crystals of the HLA-DQ2/peptide complex, which can effectively diffract X-rays for the determination of the atomic coordinates.

[32] The present invention further includes methods of using the structural information provided herein to derive a detailed structure of related peptide binding interactions, particularly other gluten peptides, or analogs and mimetics thereof. Such structural homology determination may utilize modeling, alone or in combination with structure determination.

The present invention provides three-dimensional coordinates for the HLA-DQ2/peptide complex. Such a data set may be provided in computer readable form. Methods of using such coordinates (including in computer readable form) in drug assays and drug screens as exemplified herein, are also part of the present invention. In a particular embodiment of this type, the coordinates contained in the data set can be used to identify potential modulators of the HLA-DQ2/peptide complex, including molecules that mimic the binding of the peptide to the HLA molecule, but which lack, or are substantially diminished in the ability to stimulate a T cell response.

In one embodiment, a potential agent for modulation of HLA-DQ2/peptide complex is selected by performing rational drug design with the three-dimensional coordinates determined for the crystal structures. Preferably the selection is performed in conjunction with computer modeling. Rational design may also be used in the genetic modification of immunogenic peptides by modeling the potential effect of a change in the amino acid sequence.

[35] Computer analysis may be performed with one or more of the computer programs including: GRASP, O (Jones et al. (1991) Acta Cryst. A47:110); QUANTA, CHARMM, INSIGHT, SYBYL, MACROMODEL; ICM, and CNS (Brunger et al. (1998) Acta Cryst. D54:905). In a further embodiment of this aspect of the invention, an initial drug screening assay is performed using the three-dimensional structure so obtained, preferably along with a docking computer program. Such computer modeling can be performed with one or more Docking programs such as DOC, GRAM and AUTO DOCK. See, for example, Dunbrack et al. (1997) Folding & Design 2:27-42.

[36] It should be understood that in the drug screening and protein modification assays provided herein, a number of iterative cycles of any or all of the steps may be performed to

optimize the selection. For example, assays and drug screens that monitor the activity of the T cells in the presence and/or absence of a potential inhibitor are also included in the present invention and can be employed as an assay or drug screen, usually as a single step in a multi-step protocol.

The structure of the HLA-DQ2/peptide complex is useful in the design of agents that mimic the activity and/or specificity of the binding interaction. The structures encoded by the data may be computationally evaluated for an ability to associate with chemical entities. This provides insight into an element's ability to associate with chemical entities. Chemical entities that are capable of associating with these domains may alter immunogenicity. Such chemical entities are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a graphical format. This allows visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities.

In one embodiment of the invention, an invention is provided for evaluating the ability of a chemical entity to associate with any of the molecules or molecular complexes set forth above. This method comprises the steps of employing computational means to perform a fitting operation between the chemical entity and the interacting surface of the polypeptide or nucleic acid; and analyzing the results of the fitting operation to quantify the association. The term "chemical entity", as used herein, refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes. Molecular design techniques are used to design and select chemical entities, including inhibitory compounds, capable of binding to the HLA molecule, or to the gluten peptide. Such chemical entities may interact directly with certain key features of the structure.

[39] It will be understood by those skilled in the art that not all of the atoms present in a significant contact residue need be present in a competitive binding agent. In fact, it is only those few atoms that shape the loops and actually form important contacts that are likely to be important for activity. Those skilled in the art will be able to identify these important atoms based on the structure model of the invention, which can be constructed using the structural data herein.

The design of compounds that bind to HLA-DQ2 according to this invention generally involves consideration of two factors. First, the compound must be capable of either competing for binding with an immunogenic gluten peptide; or physically and structurally associating with the HLA-DQ2 domains. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

[41] The compound must be able to assume a conformation that allows it to interact with the binding pocket. Although certain portions of the compound will not directly participate in

these associations, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of an entity comprising several interacting chemical moieties.

Computer-based methods of analysis fall into two broad classes: database methods [42] and de novo design methods. In database methods the compound of interest is compared to all compounds present in a database of chemical structures and compounds whose structure is in some way similar to the compound of interest are identified. The structures in the database are based on either experimental data, generated by NMR or x-ray crystallography, or modeled three-dimensional structures based on two-dimensional data. In de novo design methods, models of compounds whose structure is in some way similar to the compound of interest are generated by a computer program using information derived from known structures, e.g. data generated by x-ray crystallography and/or theoretical rules. Such design methods can build a compound having a desired structure in either an atomby-atom manner or by assembling stored small molecular fragments. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within the interacting surface of the RNA. Docking may be accomplished using software such as Quanta (Molecular Simulations, San Diego, CA) and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

[43] Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include: SmoG, GRID (Goodford (1985) J. Med. Chem., 28, pp. 849-857; Oxford University, Oxford, UK; MCSS (Miranker et al. (1991) Proteins: Structure, Function and Genetics, 11, pp. 29-34; Molecular Simulations, San Diego, CA); AUTODOCK (Goodsell et al., (1990) Proteins: Structure, Function, and Genetics, 8, pp. 195-202; Scripps Research Institute, La Jolia, Calif.); and DOCK (Kuntz et al. (1982) J. Mol. Biol., 161:269-288; University of California, San Francisco, Calif.)

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates. Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett et al. (1989) In Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196; University of California, Berkeley, Calif.); 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif); and HOOK (available from Molecular Simulations, San Diego, CA).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., N. C. Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990). See also, M. A. Navia et al., "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once the binding entity has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit by the same computer methods described above.

Another approach made possible and enabled by this invention, is the computational screening of small molecule databases. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy. Generally the tighter the fit, the lower the steric hindrances, and the greater the attractive forces, the more potent the potential modulator since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug the more likely that the drug will not interact as well with other proteins. This will minimize potential side effects due to unwanted interactions with other proteins.

Compounds of interest can be systematically modified by computer modeling programs until one or more promising potential analogs are identified. In addition systematic modification of selected analogs can then be systematically modified by computer modeling programs until one or more potential analogs are identified. Alternatively a potential modulator could be obtained by initially screening a random peptide library, for example one produced by recombinant bacteriophage. A peptide selected in this manner would then be systematically modified by computer modeling programs as described above, and then treated analogously to a structural analog.

Once a potential modulator/inhibitor is identified it can be either selected from a library of chemicals as are commercially available from most large chemical companies including Merck, GlaxoWelcome, Bristol Meyers Squib, Monsanto/Searle, Eli Lilly, Novartis and Pharmacia UpJohn, or alternatively the potential modulator may be synthesized *de novo*. The *de novo* synthesis of one or even a relatively small group of specific compounds is reasonable in the art of drug design.

[50] The success of both database and *de novo* methods in identifying compounds with activities similar to the compound of interest depends on the identification of the functionally

relevant portion of the compound of interest. For drugs, the functionally relevant portion may be referred to as a pharmacophore, *i.e.* an arrangement of structural features and functional groups important for biological activity. Not all identified compounds having the desired pharmacophore will act as a modulator of inflammation. The actual activity can be finally determined only by measuring the activity of the compound in relevant biological assays. However, the methods of the invention are extremely valuable because they can be used to greatly reduce the number of compounds that must be tested to identify an actual inhibitor.

In order to determine the biological activity of a candidate pharmacophore it is preferable to measure biological activity at several concentrations of candidate compound. The activity at a given concentration of candidate compound can be tested in a number of ways.

[52] For example, an HLA molecule can be attached to a solid support. Methods for placing proteins on a solid support are well known in the art and include such steps as linking biotin to the protein, and linking avidin to the solid support. The solid support can be washed to remove unreacted species. A solution of a labeled candidate agent can be contacted with the solid support. The solid support is washed again to remove the potential modulator not bound to the support. The amount of labeled potential modulator remaining with the solid support and thereby bound to the protein can be determined. Alternatively, or in addition, the dissociation constant between the labeled candidate agent and the protein can be determined.

Crystals of the binding complex of the present invention can be grown by a number of techniques including batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and by microdialysis. Seeding of the crystals in some instances is required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used. The crystals may be shrunk by transfer into solutions of different composition, e.g. by the addition of metal ions such as Mn<sup>2+</sup>, Pb<sup>2+</sup>, etc. Crystals may also be generated that include cofactors, substrates, candidate inhibitors, and the like, that interact with the protein, e.g. by cocrystallization of soaking protein crystals in a solution comprising an inhibitor or other agent.

by using X-rays produced in a conventional source (such as a sealed tube or a rotating anode) or using a synchrotron source. Methods of characterization include, but are not limited to, precision photography, oscillation photography and diffractometer data collection. Selenium-methionine may be used as described in the examples provided herein, or alternatively a heavy metal derivative data set (e.g., using PCMB) may be used in place of the selenium-methionine derivatization.

Electron density maps may be built from crystals using phase information from multiple isomorphous heavy-atom derivatives, molecular replacement or selenomethionine incorporated multiwavelength anomalous disperson technique. Model building is facilitated by the use of sequence markers, especially selenomethionine residues. Anomalous difference Fourier maps may be calculated with data from selenomethionine-substituted HLA-DQ2/ GLUTEN EPITOPE and with experimental multiple isomorphous replacement with anomalous scattering (MIRAS) phases (Hemming and Edwards (2000) J. Biol. Chem. 275:2288). Maps are improved by phase combination, where MIRAS phases are combined by the program SIGMAA (Jones et al., supra.) Phase combination may be followed by solvent flattening with DM (Carson (1997) Methods Enzymol. 277:493). Improved maps may be obtained by combination of the MIRAS phases with improved phases from combined polyalanine and atomic models in an iterative process. The model can be refined by classical positional and B-factor minimization, and with manual rebuilding.

HLA-DQ2/peptide complex structure models and databases of structure information are provided. The structural models find use in determining the structure of related and/or analogous peptide complexes. In some cases, modeling will be based on the provided structure. In other embodiments, modeling will utilize the provided structure in combination with features present in homologous and/or related structures, where relationship may be defined by protein sequence similarity, or structural similarity, e.g. in the presence of specific features as described above.

[56]

The structure model may be implemented in hardware or software, or a combination of both. For most purposes, in order to use the structure coordinates generated for the structure, it is necessary to convert them into a three-dimensional shape. This is achieved through the use of free or commercially available software that is capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structure coordinates.

In one embodiment of the invention, a machine-readable storage medium is provided, the medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of any of the structures of this invention that have been described above. Specifically, the computer-readable storage medium is capable of displaying a graphical three-dimensional representation of the HLA-DQ2/peptide complex.

[59] Thus, in accordance with the present invention, data providing structural coordinates, alone or in combination with software capable of displaying the resulting three dimensional structure of the complex, portions thereof, and their structurally similar analogs, is stored in a machine-readable storage medium. Such data may be used for a variety of

purposes, such as drug discovery, analysis of interactions between cellular components during translation, modeling of vaccines, and the like.

Preferably, the invention is implemented in computer programs executing on programmable computers, comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

[61] Each program is preferably implemented in a high level procedural or object oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

[62] Each such computer program is preferably stored on a storage media or device (e.g., ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

The HLA-binding peptide inhibitors are incorporated into a variety of formulations for therapeutic administration. In one aspect, the agents are formulated into pharmaceutical compositions by combination with appropriate, pharmaceutically acceptable carriers or diluents, and may be formulated into preparations in solid, semi-solid, liquid or gaseous forms, such as tablets, capsules, powders, granules, ointments, solutions, suppositories, injections, inhalants, gels, microspheres, and aerosols. As such, administration can be achieved in various ways, usually by oral administration. The HLA-binding peptide inhibitors may be systemic after administration or may be localized by virtue of the formulation, or by the use of an implant that acts to retain the active dose at the site of implantation.

In pharmaceutical dosage forms, the HLA-binding peptide inhibitors may be administered in the form of their pharmaceutically acceptable salts, or they may also be used alone or in appropriate association, as well as in combination with other pharmaceutically active compounds. The agents may be combined, as previously described, to provide a cocktail of activities. The following methods and excipients are merely exemplary and are in no way limiting.

[65] For oral preparations, the agents can be used alone or in combination with appropriate additives to make tablets, powders, granules or capsules, for example, with conventional additives, such as lactose, mannitol, corn starch or potato starch; with binders, such as crystalline cellulose, cellulose derivatives, acacia, corn starch or gelatins; with disintegrators, such as corn starch, potato starch or sodium carboxymethylcellulose; with lubricants, such as talc or magnesium stearate; and if desired, with diluents, buffering agents, moistening agents, preservatives and flavoring agents.

In one embodiment of the invention, the oral formulations comprise enteric coatings, so that the active agent is delivered to the intestinal tract. Enteric formulations are often used to protect an active ingredient from the strongly acid contents of the stomach. Such formulations are created by coating a solid dosage form with a film of a polymer that is insoluble in acid environments, and soluble in basic environments. Exemplary films are cellulose acetate phthalate, polyvinyl acetate phthalate, hydroxypropyl methylcellulose phthalate and hydroxypropyl methylcellulose acetate succinate, methacrylate copolymers, and cellulose acetate phthalate.

Other enteric formulation comprise engineered polymer microspheres made of biologically erodable polymers, which display strong adhesive interactions with gastrointestinal mucus and cellular linings, can traverse both the mucosal absorptive epithelium and the follicle-associated epithelium covering the lymphoid tissue of Peyer's patches. The polymers maintain contact with intestinal epithelium for extended periods of time and actually penetrate it, through and between cells. See, for example, Mathiowitz et al. (1997) Nature 386 (6623): 410-414. Drug delivery systems can also utilize a core of superporous hydrogels (SPH) and SPH composite (SPHC), as described by Dorkoosh et al. (2001) J Control Release 71(3):307-18.

[68] Formulations are typically provided in a unit dosage form, where the term "unit dosage form," refers to physically discrete units suitable as unitary dosages for human subjects, each unit containing a predetermined quantity of glutenase calculated in an amount sufficient to produce the desired effect in association with a pharmaceutically acceptable diluent, carrier or vehicle. The specifications for the unit dosage forms of the present invention depend on the particular complex employed and the effect to be achieved, and the pharmacodynamics associated with each complex in the host.

The pharmaceutically acceptable excipients, such as vehicles, adjuvants, carriers or diluents, are readily available to the public. Moreover, pharmaceutically acceptable auxiliary substances, such as pH adjusting and buffering agents, tonicity adjusting agents, stabilizers, wetting agents and the like, are readily available to the public.

[69]

### METHODS OF TREATMENT

The subject methods are used to treat individuals suffering from Celiac Sprue and/or dematitis herpetiformis, by administering an effective dose through a pharmaceutical formulation. Diagnosis of suitable patients may utilize a variety of criteria known to those of skill in the art. A quantitative increase in antibodies specific for gliadin, and/or tissue transglutaminase is indicative of the disease. Family histories and the presence of the HLA alleles HLA-DQ2 [DQ(a1\*05, b1\*02)] and/or DQ8 [DQ(a1\*03, b1\*0302)] are indicative of a susceptibility to the disease. Specific peptide analogs may be administered therapeutically to decrease inflammation, and/or to induce antigen-specific tolerance to treat autoimmunity. Methods for the delivery of peptides that are altered from a native peptide are known in the art. Alteration of native peptides with selective changes of crucial residues can induce unresponsiveness or change the responsiveness of antigen-specific autoreactive T cells.

[71] The therapeutic effect may be measured in terms of clinical outcome, or may rely on immunological or biochemical tests. Suppression of the deleterious T-cell activity can be measured by enumeration of reactive Th1 cells, by quantitating the release of cytokines at the sites of lesions, or using other assays for the presence of autoimmune T cells known in the art. Alternatively, one may look for a reduction in symptoms of a disease.

Various methods for administration may be employed. The dosage of the therapeutic formulation will vary widely, depending upon the nature of the disease, the frequency of administration, the manner of administration, the clearance of the agent from the host, and the like. Such treatment could either be before meals or on a once-a-day basis or on a once-a-week basis, depending on the half-life of the inhibitor. A typical dose is at least about 1 μg, usually at least about 10 μg, more usually at least about 0.1 mg, and not more than about 10 mg, usually not more than about 1 mg. Enteric coating of these peptides may also enhance their lifetimes in the gut, thereby permitting delivery to the proximal and distal small intestinal tissue. Treatment of other autoimmune disorders such as Type I diabetes with such ligands may involve oral, intravenous or intramuscular administration. The initial dose may be larger, followed by smaller maintenance doses. The dose may be administered as infrequently as weekly or biweekly, or more often fractionated into smaller doses and administered daily, with meals, semi-weekly, *etc.* to maintain an effective dosage level.

The HLA-binding peptide inhibitors of the invention may be administered in the treatment of Type 1 diabetes (IDDM). IDDM and celiac disease are both immunologic disorders where specific HLA alleles are associated with disease risk. Transglutaminase autoantibodies can be found in some patients with IDDM. The prevalence of transglutaminase autoantibodies is higher in diabetic patients with HLA DQ2 or DQ8.

Human type I or insulin-dependent diabetes mellitus (IDDM) is characterized by autoimmune destruction of the β cells in the pancreatic islets of Langerhans. The depletion of β cells results in an inability to regulate levels of glucose in the blood. Overt diabetes occurs when the level of glucose in the blood rises above a specific level, usually about 250 mg/dl. In humans a long presymptomatic period precedes the onset of diabetes. During this period there is a gradual loss of pancreatic beta cell function. IDDM is currently treated by monitoring blood glucose levels to guide injection, or pump-based delivery, of recombinant insulin. Diet and exercise regimens contribute to achieving adequate blood glucose control. The inhibitors of the invention may be administered alone, or in combination with other therapies. The route of administration may be oral, as described for treatment of Celiac Sprue, or may be injected, e.g. i.v., i.m., etc. Administration may be performed during the pre-symptomatic phase, or in overt diabetes.

#### **EXPERIMENTAL**

#### Example

It has long been known that the principal toxic components of wheat gluten are a family of closely related Pro-Gln rich proteins called gliadins. Recent reports have suggested that peptides from a short segment of α-gliadin appear to account for most of the gluten-specific recognition by CD4+ T cells from Celiac Sprue patients. These peptides are substrates of tissue transglutaminase (tTGase), the primary auto-antigen in Celiac Sprue, and the products of this enzymatic reaction bind to the class II HLA DQ2 molecule. This "immunodominant" region of α-gliadin is part of an unusually long proteolytic product generated by the digestive process that: (a) is exceptionally resistant to further breakdown by gastric, pancreatic and intestinal brush border proteases; (b) is the highest specificity substrate of human tissue transglutaminase (tTGase) discovered to date; (c) contains at least six overlapping copies of epitopes known to be recognized by patient derived T cells; (d) stimulates representative T cell clones that recognize these epitopes with submicromolar efficacy; and (e) has homologs in proteins from all toxic foodgrains but no homologs in non-toxic foodgrain proteins.

Identification of stable peptides from gastric protease, pancreatic protease and brush border membrane peptidase catalyzed digestion of recombinant α2-gliadin: α2-gliadin, a representative α-gliadin (Arentz-Hansen et al. (2000) Gut 46:46), was expressed in recombinant form and purified from E. coli. The α2-gliadin gene was cloned in pET28a plasmid (Novagen) and transformed into the expression host BL21(DE3) (Novagen). The transformed cells were grown in 1-liter cultures of LB media containing 50 μg/ml of

kanamycin at 37 °C until the OD600 0.6-1 was achieved. The expression of α2-gliadin protein was induced with the addition of 0.4 mM isopropyl  $\alpha$ -D-thiogalactoside (Sigma) and the cultures were further incubated at 37 °C for 20 hours. The cells expressing the recombinant α2-gliadin were centrifuged at 3600 rpm for 30 minutes. The pellet was resuspended in 15 ml of disruption buffer (200 mM sodium phosphate; 200 mM NaCl; 2.5 mM DTT; 1.5 mM benzamidine; 2.5 mM EDTA; 2 mg/L pepstatin; 2 mg/L leupeptin; 30% v/v glycerol) and lysed by sonication (1 minute; output control set to 6). After centrifugation at 45000g for 45 min, the supernatant was discarded and the pellet containing gliadin protein was resuspended in 50 ml of 7M urea in 50 mM Tris (pH = 8.0). The suspension was again centrifuged at 45000g for 45 min and the supernatant was harvested for purification. The supernatant containing α2-gliadin was incubated with 1 ml of nickel-nitrilotriacetic acid resin (Ni-NTA; Qiagen) overnight and then batch-loaded on a column with 2 ml of Ni-NTA. The column was washed with 7M urea in 50 mM Tris (pH = 8.0) and  $\alpha$ 2-gliadin was eluted with 200 mM imidazole, 7 M urea in 50 mM Tris (pH = 4.5). The fractions containing  $\alpha$ 2-gliadin were pooled into a final concentration of 70% ethanol solution and two volumes of 1.5M NaCl were added to precipitate the protein. The solution was incubated at 4 °C overnight and the final precipitate was collected by centrifugation at 45000 g for 30 min, rinsed in water, and re-centrifuged to remove the urea. The final purification step of the α-2 gliadin was developed with reverse-phase HPLC. The Ni-NTA purified protein fractions were pooled in 7 M urea buffer and injected to a Vydac (Hesperia, CA) polystyrene reversephase column (i.d. 4.6 mm × 25 cm) with the starting solvent (30% of solvent B: 1:1 HPLCgrade acetonitrile/isopropanol: 0.1% TFA). Solvent A was an aqueous solution with 0.1% TFA. The separation gradient extended from 30–100% of solvent B over 120 min at a flow rate of 0.8 ml/min.

Table 2, Amount of Peptides Digested after 15 hours

	33-mer	Control A	Control B
H1P0	<20%	>90%	>90%
H2P0	<20%	>61%	>85%
H3P0	<20%	>87%	>95%
H4P0	<20%	>96%	>95%
H5P0	<20%	>96%	>95%

The purity of the recombinant gliadin was >95%, which allowed for facile identification and assignment of proteolytic products by LC-MS/MS/UV. Although many previous studies utilized pepsin/trypsin treated gliadins, it was found that, among gastric and pancreatic proteases, chymotrypsin played a major role in the breakdown of α2-gliadin,

resulting in many small peptides from the C-terminal half of the protein and a few longer (>8 residues) peptides from the N-terminal half, the most noteworthy being a relatively large fragment, the 33-mer LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQPQF (residues 57-89). This peptide was of particular interest for two reasons: (a) Whereas most other relatively stable proteolytic fragments were cleaved to smaller fragments when the reaction times were extended, the 33-mer peptide remained intact despite prolonged exposure to proteases; and (b) three distinct patient-specific T cell epitopes identified previously are present in this peptide, namely, PFPQPQLPY, PQPQLPYPQ (3 copies), and PYPQPQLPY (2 copies).

To establish the physiological relevance of this peptide, composite gastric/pancreatic enzymatic digestion of α2 gliadin was then examined. As expected, enzymatic digestion with pepsin (1:100 w/w ratio), trypsin (1:100), chymotrypsin (1:100), elastase (1:500) and carboxypeptidase (1:100) was quite efficient, leaving behind only a few peptides longer than 9 residues (the minimum size for a peptide to show class II MHC mediated antigenicity). In addition to the above-mentioned 33-mer, the peptide WQIPEQSR was also identified, and was used as a control in many of the following studies.

[79]

#### Example 2

The 33-mer gliadin peptide is an excellent substrate for tTGase, and the resulting product is a highly potent activator of patient-derived T cells: A number of recent studies have demonstrated that regiospecific deamidation of immunogenic gliadin peptides by tTGase increases their affinity for HLA-DQ2 as well as the potency with which they activate patient-derived gluten-specific T cells. It has been shown the specificity of tTGase for certain short antigenic peptides derived from gliadin is higher than its specificity toward its physiological target site in fibronectin, for example, the specificity of tTGase for the α-gliadin

Structural characteristics of the 33-mer gliadin peptide and its naturally occurring [81] homologs: Sequence alignment searches using BLASTP in all non-redundant protein databases revealed several homologs (E-value < 0.001) of the 33-mer gliadin peptide. Interestingly, foodgrain derived homologs were only found in gliadins (from wheat), hordeins (from barley) and secalins (from rye), all of which have been proven to be toxic to Celiac patients (Figure 7). Nontoxic foodgrain proteins, such as avenins (in oats), rice and maize, do not contain homologous sequences to the 33-mer gliadin. In contrast, a BLASTP search with the entire  $\alpha$ 2-gliadin sequence identified foodgrain protein homologs from both toxic and nontoxic proteins. Based on available information regarding the substrate specificities of gastric, pancreatic and BBM proteases and peptidases, it is predicted that, although most gluten homologs to the 33-mer gliadin peptide contained multiple proteolytic sites and are therefore unlikely to be completely stable toward digestion, several sequences from wheat, rye and barley are expected to be comparably resistant to gastric and intestinal proteolysis. The stable peptide homologs to the 33-mer a2-gliadin peptide are OPOPFPPOLPYPOTOPFPPOOPYPQPQPQPQPQQ (from  $\alpha$ 1- and  $\alpha$ 6-gliadins); QQQPFPQQPIPQQPQPYPQQPQPYPQQPFPPQQPF (from B1 hordein); QPFPQPQQTFPQQPQLPFPQQPQQPFPQPQ (from y-gliadin); VQWPQQQPVPQPHQPF (from γ-gliadin), VQGQGIIQPQQPAQ (from γ-gliadin), FLQPQQPFPQQPQQPYPQQPQQPFPQ (from  $\gamma$ -gliadin), FSQPQQQFPQPQQPQQSFPQQQPP (from  $\gamma$ -gliadin), QPFPQPQQPTPIQPQQPFPQRPQQPFPQPQ (from  $\omega$ -secalin). These stable peptides are all located at the N-terminal region of the corresponding proteins. The presence of proline residues after otherwise cleavable residues in these peptides would contribute to their proteolytic stability.

The unique primary sequence of the 33-mer gliadin peptide also had homologs among a few non-gluten proteins. Among the strongest homologs were internal sequences from pertactin (a highly immunogenic protein from *Bordetella pertussis*) and a mammalian inositol-polyphosphate 5-phosphatase of unknown function. In both cases available information suggested that the homology could have biologically relevance. For example, the region of pertactin that is homologous to the 33-mer gliadin peptide is known to be part of the immunodominant segment of the protein. In the case of the homologous phosphatase, the corresponding peptide region of the phosphatase is known to be responsible for vesicular trafficking of the phosphatase to the cytoplasmic Golgi. In analogy with the current picture of how gliadin peptides are presented to HLA-DQ2 via a tTGase mediated pathway, these Pro-Gln-rich segments of both pertactin and the phosphatase are likely to be good tTGase substrates.

## Example 3

[83] X-ray Crystallographic Analysis of soluble HLA-DQ2. The soluble extracellular domains of the  $\alpha$ - and  $\beta$ -chains of HLA-DQ2 were co-expressed in insect cells using a baculovirus expression system (pAcAB3 vector, BD Biosciences). The DNA sequence of the engineered  $\alpha$ - and  $\beta$ -chains is provided in SEQ ID NO:1 and SEQ ID NO:2. The  $\beta$ -chain is fused to a sequence encoding the epitope QLQPFPQPELPY at its N-terminal end, and to a biotin recognition sequence at its C-terminal end. Both subunits are also fused to complementary leucine zipper sequences at their C-terminal ends. Since a Factor Xa proteolysis site is engineered between the leucine zipper sequences and the DQ2 subunits, prior to crystallization the leucine zippers were removed from DQ2 by Factor Xa digestion.

[84]

Initial purification of the DQ2 heterodimer from the culture medium was performed on an immunoaffinity column containing an anti-DQ2 monoclonal antibody (2.12.E11) bound to a Protein A Sepharose CL-4B column. Subsequently DQ2 was treated with Factor Xa, and purified from the digestion mixture by anion-exchange chromatography followed by size-exclusion chromatography, and concentrated to 4 mg/ml in 25 mM Tris-HCl, pH 8.0. Crystals of the DQ2-epitope complex were obtained using the hanging drop method. Typically, 2  $\mu$ L of protein solution (2~4 mg/ml DQ2, 25 mM Tris-HCl, pH 8.0) and 2  $\mu$ L of precipitant buffer (200 mM ammonium acetate, 40 mM ammonium sulfate, 4% ethylene glycol, 22~26% PEG 3350) were combined in a single drop hanging over 1 mL of precipitant buffer at room temperature. Small crystals appeared within three days and grew to full size in two weeks.

[85] For data collection, crystals were transferred to a cryoprotectant solution (mother liquor containing 28% ethylene glycol) for 2 hours, and then flash cooled at 100K in liquid nitrogen. X-ray diffraction data were collected from a single crystal to 2.22 Å resolution at

beamline 11-1 of the Stanford Synchrotron Radiation Laboratory using a Quantum 315 CCD detector. Oscillation images were processed with DENZO and data reduction was carried out with SCALEPACK.

The structure of DQ2-epitope complex was determined by molecular replacement using the program AMoRe in the CCP4 suite of programs. The 2.4 Å resolution structure of insulin peptide-HLA-DQ8 complex (RCSB accession code: 1JK8) minus the insulin peptide and solvent molecules was used as the search model. After initial refinement with the maximum likelihood function of program REFMAC, iterative cycles of refinement including simulated annealing, temperature factor refinement, and energy minimization were made with the program CNS. Model building and correction were performed using  $\sigma_A$ -weighted  $F_o$ - $F_c$  and  $2F_o$ - $F_c$  electron density maps with the program O. The current model has R-factor of 0.2209 with a  $R_{\rm free}$  of 0.2793 at 2.22 Å resolution. Analysis of the Ramachandran plot generated using the program PROCHECK shows that 91.2 % of residues are in most favored regions, 7.9 % are in additional allowed regions, 0.5 % are in generously allowed regions, and 0.5 % are in disallowed regions.

There are two molecules of DQ2-epitope in the asymmetric unit. In the first complex,  $\alpha$ -chain of DQ2,  $\beta$ -chain of DQ2, and the alpha-I epitope peptide (sequence QLQPFPQPELPY) are designated A, B, and C respectively. In the second complex,  $\alpha$ -chain,  $\beta$ -chain, and epitope peptide are designated D, E, and F respectively. The model includes 354 water molecules (name: HOH) and 4 ethylene glycol molecules (name: EDO).

Thr-106—His-112 region in chain B and Arg-105—His-112 region in chain E are disordered and thus absent from the model. Superposition of the DQ8 structure suggests that these regions form an extended loop. Side chain conformation of the following residues are undefined due to weak electron density in the corresponding region and therefore only their backbone atoms are included in the model: Asp-135 (in chain B), Leu-2, Gln-3, Tyr-12 (in chain C), Asp-135, Gln-136 (in chain E), and Leu-2, Gln-3 (in chain F).

Structure-based design of DQ2 binding peptide inhibitors. The crystal structure of the DQ2-epitope complex reveals precisely which atoms in the peptide QLQPFPQPELPYP point outward (by inference into the T cell receptor binding pocket). Substitutions at these atoms can yield altered peptide ligands that retain the ability to bind tightly to DQ2 but are no longer able to allow docking of the DQ2-peptide complex into disease specific T cell receptors.

The coordinate of the structure are as follows:

[88]

[89]

[90]

#### Coordinates

REMARK peptide link removed (applied DPEP): from B 105 to B 113
REMARK peptide link removed (applied DPEP): from E 104 to E 113
REMARK disulphide added: from A 107 to A 163
REMARK disulphide added: from B 15 to B 79
REMARK disulphide added: from B 117 to B 173

REMARK	disulp	hide	add	led:	from	D	107	to D	163			
REMARK	-						15	to E	79 172			
REMARK REMARK	_				110m 3:00:6		117 'C	to E reated by	173 v user:	kim		
REMARK				_		-	•		,			
ATOM	1	CB	VAL		2		31.060	3.851	4.095		39.43	A
ATOM	2		VAL		2		30.078	2.835	3.531		40.06	A A
ATOM ATOM	3 4	CG2	VAL VAL		2 2		30.370 30.653	5.185 3.406	4.344 6.542		39.97 36.80	A
ATOM	5	o	VAL		2		29.644	2.702	6.527		38.25	A
MOTA	6	N	VAL		2		32.189	1.926	5.235		36.80	A
ATOM	7	CA	VAL		2		31.684	3.321	5.414		37.95	A
ATOM	8	N	ALA		3		30.910	4.267	7.523		34.99	A
ATOM ATOM	9 10	CA CB	ALA ALA		3 3		30.003	4.416 3.368	8.658 9.721		32.94 33.34	A A
ATOM	11	C	ALA		3		30.094	5.805	9.263		30.81	A
ATOM	12	0	ALA		3		30.980	6.583	8.914	1.00	29.57	A
ATOM	13	N	ASP		4		29.172	6.115	10.170		28.70	A
MOTA	14	CA	ASP		4		29.173	7.416	10.822		26.95	A
ATOM ATOM	15 16	CB CG	ASP ASP		4 4		27.812 26.687	7.722 7.845	11.456 10.431		28.65 31.67	A A
ATOM	17		ASP		4		26.904	8.417	9.339		33.31	A
ATOM	18		ASP		4		25.568	7.381	10.735		33.31	A
MOTA	19	C	ASP		4		30.254	7.432	11.898		26.51	A
ATOM	20	0	ASP		4		30.857	8.469	12.170		25.25	A
ATOM	21	N	HIS		5 5		30.493 31.527	6.277 6.164	12.515 13.544		26.22 26.52	A A
ATOM ATOM	22 23	CA. CB	HIS		5		30.939	6.339	14.950		25.34	A
ATOM	24	CG	HIS		5		30.240	7.647	15.156		28.69	A
ATOM	25	CD2	HIS	A	5		30.716	8.870	15.492		29.15	A
MOTA	26		HIS		5		28.881	7.801	14.979		28.23	A
ATOM	27		HIS		5 5		28.550	9.062 9.732	15.198 15.511		29.92 29.84	A A
ATOM ATOM	28 29	C N⊞3	HIS		5		29.645 32.246	4.826	13.465		25.79	A
ATOM	30	ō	HIS		5		31.630	3.785	13.227		25.68	A
ATOM	31	N	VAL		6		33.559	4.866	13.659	1.00	24.52	A
MOTA	32	CA	VAL		6		34.385	3.667	13.628		23.27	A
ATOM	33	CB	VAL		6 6		35.311	3.657 2.414	12.407 12.440		25.22 24.31	A A
ATOM ATOM	34 35		VAL		6		36.187 34.489	3.708	11.127		27.15	A
ATOM	36	C	VAL		6		35.256	3.633	14.876		22.15	A
ATOM	37	0	VAL	A	6		35.937	4.606	15.185		21.49	A
ATOM	38	N	ALA		7		35.239	2.513	15.586		19.90	A
ATOM	39 40	CA CB	ALA ALA		7 7		36.038 35.132	2.382 2.394	16.799 18.034		19.70 14.59	A A
MOTA MOTA	41	C	ALA		7		36.867	1.111	16.791		18.62	A
ATOM	42	ō	ALA		7		36.548	0.153	16.088	1.00	20.78	A
ATOM	43	N	SER	A	8		37.947	1.120	17.560		16.95	A
MOTA	44	CA	SER		8		38.807	-0.048	17.700		18.62	A
ATOM ATOM	45 46	CB OG	SER SER		8 8		40.211 40.209	0.215 0.271	17.153 15,738		17.69 19.81	A A
MOTA	47	C	SER		8		38.868	-0.310	19.199		18.76	A
MOTA	48	ō	SER		8		39.570	0.376	19.943		19.35	A
MOTA	49	N	TYR		9		38.070	-1.268	19.645		19.38	A
ATOM	50	CA	TYR		9		38.038	-1.608	21.048 21.471		19.44 19.18	A A
ATOM ATOM	51 52	CB	TYR TYR		9 9		36.628 35.714	-1.980 -0.785	21.375		18.65	A
ATOM	53		TYR		9		36.073	0.435	21.962		16.57	A
MOTA	54	CE1	TYR	A	9		35.237	1.537	21.897		17.39	A
MOTA	55		TYR		9		34.493	-0.865	20.716		17.15	A
MOTA	56		TYR		9		33.641 34.020	0.235 1.431	20.647 21.243		16.82 18.07	A A
MOTA MOTA	57 58	CZ	TYR TYR		9 9		33.169	2.509	21.210		19.77	A
MOTA	59	C	TYR		9		38.993	-2.751	21.106		20.21	A
ATOM	60	0	TYR	A	9		38.652	-3.911	21.344		15.05	A
ATOM	61	N	GLY		10		40.225	-2.357	20.831		21.69	A
ATOM	62 63	CA	GLY		10		41.311	-3.275 -3.080	20.808 19.655		22.54 21.74	A A
MOTA MOTA	63 64	0	GLY GLY		10 10		42.248	-3.863	18.713		22.02	A
ATOM	65	N	VAL		11		43.083	-2.023	19.674	1.00	18.91	A
MOTA	66	CA	VAL	A	11		44.119	-1.949	18.651		17.39	A
ATOM	67	CB	VAL		11		44.554	-0.506	18.277		18.75 16.18	A A
MOTA MOTA	68 69		VAL VAL		11 11		45.845 43.481	-0.558 0.165	17.455 17.432		15.25	A
	35									_,		

									_
ATOM	70	С	VAL A		45.228	-2.644	19.447	1.00 17.05	A
ATOM	71	0	VAL A		45.679	-2.145	20.481	1.00 19.34	A
MOTA	72	N	ASN A	12	45.616	-3.828	19.005	1.00 17.39	A
ATOM	73	CA	ASN A	12	46.643	-4.597	19.693	1.00 17.18	A
MOTA	74	СВ	ASN A	12	46.113	-5.994	20.052	1.00 15.04	A
ATOM	75	CG	ASN A		44.834	-5.947	20.882	1.00 15.96	A
						-5.490		1.00 18.20	A
MOTA	76		ASN A		43.780		20.417		
MOTA	77	ND2	ASN A		44.921	-6.420	22.114	1.00 10.46	A
ATOM	78	C	ASN A	12	47.863	-4.739	18.797	1.00 18.90	A
ATOM	79	0	ASN A	. 12	47.752	-5.162	17.641	1.00 18.80	A
ATOM	80	N	LEU A	13	49.026	-4.403	19.343	1.00 18.60	A
ATOM	81	CA	LEU A		50.264	-4.478	18.599	1.00 19.90	A
	82	CB	LEU A		50.695	-3.064	18.217	1.00 23.26	A
ATOM								1.00 24.86	A
ATOM	83	CG	LEU A		52.077	-2.881	17.594		
MOTA	84		LEU A		52.085	-3.494	16.201	1.00 26.92	A
ATOM	85	CD2	LEU A	. 13	52.417	-1.402	17.534	1.00 24.75	A
ATOM	86	C	TEG Y	. 13	51.391	-5.165	19.370	1.00 20.37	A
ATOM	87	0	LEU A	. 13	51.559	-4.953	20.566	1.00 21.11	A
MOTA	88	N	TYR A	14	52.145	-6.004	18.673	1.00 21.04	A
ATOM	89	CA	TYR A		53.291	-6.691	19.255	1.00 24.07	A
		СВ	TYR A		52.909	-8.050	19.844	1.00 27.05	A
ATOM	90							1.00 29.27	A
ATOM	91	CG	TYR A		54.091	-8.729	20.489		
ATOM	92		TYR A		54.569	-8.304	21.723	1.00 30.07	A
ATOM	93	CE1	TYR A	14	55.709	-8.867	22.285	1.00 31.38	A
ATOM	94	CD2	TYR A	14	54.783	-9.744	19.830	1.00 31.63	A
ATOM	95	CE2	TYR A	14	55.923	-10.314	20.383	1.00 30.29	A
MOTA	96	CZ	TYR A		56.381	-9.868	21.609	1.00 31.37	A
	97	OH	TYR A			-10.413	22.160	1.00 34.48	A
ATOM					54,291	-6.900	18.128	1.00 25.30	A
ATOM	98	C	TYR A					1.00 25.50	
MOTA	99	0	TYR F		53.907	-7.206	16.994		A
MOTA	100	N	GLN A	15	55.571	-6.725	18.429	1.00 24.61	A
ATOM	101	CA	GLN A	15	56.603	-6.891	17.414	1.00 25.19	A
ATOM	102	CB	GLN A	15	56.932	-5.549	16.754	1.00 23.54	A
ATOM	103	CG	GLN A		57.278	-4.443	17.738	1.00 23.98	A
ATOM	104	CD	GLN A		57.567	-3.116	17.056	1.00 26.32	A
					57.575	-2.062	17.702	1.00 28.26	A
MOTA	105	OE1						1.00 24.64	A
MOTA	106	NE2			57.810	-3.159	15.749		
ATOM	107	C	GLN A	1 15	57.848	-7.487	18.036	1.00 26.16	A
MOTA	108	0	GLN A	1 15	58.134	-7.263	19.211	1.00 24.31	A
MOTA	109	N	SER A	1 16	58.583	-8.252	17.236	1.00 28.72	A
ATOM	110	CA	SER A	16	59.801	-8.912	17.698	1.00 30.37	A
ATOM	111	CB	SER A		60.341	-9.830	16.603	1.00 28.35	A
			SER A		60.569	-9.100	15.407	1.00 31.43	A
MOTA	112	OG						1.00 32.37	A
MOTA	113	С	SER 1		60.883	-7.918	18.111		
MOTA	114	0	SER 1		61.538	-8.104	19.134	1.00 33.91	A
MOTA	115	N	TYR I	A 17	61.073	-6.863	17.325	1.00 32.49	A
ATOM	116	CA	TYR Z	A 17	62.096	-5.890	17.664	1.00 34.27	A
ATOM	117	CB	TYR I	A 17	62.172	-4.788	16.620	1.00 35.41	A
ATOM	118	CG	TYR I		63.371	-3.911	16.837	1.00 37.77	A
ATOM	119		TYR		64.646	-4.347	16.470	1.00 39.38	A
			TYR		65.769	-3.569	16.715	1.00 40.15	A
MOTA	120							1.00 36.31	A
MOTA	121		TYR		63.247	-2.671	17.456		
ATOM	122		TYR		64.360	-1.886	17.707	1.00 39.40	A
MOTA	123	CZ	TYR .	A 17	65.621	-2.338	17.335	1.00 41.42	A
ATOM	124	OH	TYR :	A 17	66.732	-1.562	17.580	1.00 43.02	A
MOTA	125	C	TYR :	A 17	61.821	~5.270	19.027	1.00 34.43	A
ATOM	126	0	TYR		60.765	-4.682	19.248	1.00 35.58	A
ATOM	127	N	GLY		62.783	-5.390	19.935	1.00 34.98	A
					62.609	-4.854	21,270	1.00 35.78	A
ATOM	128	CA	GLY .				22,292	1.00 36.87	A
MOTA	129	С	GLY .		62.730	-5.968			
MOTA	130	0	GLY .		63.761	-6.082	22.952	1.00 38.48	A
MOTA	131	N	PRO .	A 19	61.692	-6.807	22.459	1.00 37.06	A
MOTA	132	CD	PRO	A 19	61.745	-7.967	23.368	1.00 35.58	A
MOTA	133	CA	PRO		60.409	-6.769	21.747	1.00 34.79	A
MOTA	134	CB	PRO		59.853	-8.166	21.981	1.00 35.91	A
			PRO		60.300	-8.437	23.394	1.00 36.88	A
MOTA	135	CG			59.531	-5.706	22.379	1.00 33.10	A
MOTA	136	C	PRO					1.00 33.71	A
MOTA	137	0	PRO		59.844	-5.209	23.456		
ATOM	138	N	SER		58.435	-5.349	21.722	1.00 31.83	A
MOTA	139	CA	SER	A 20	57.548		22.290	1.00 30.25	A
ATOM	140	CB	SER	A 20	58.060	-2.932	21.965	1.00 29.00	A
ATOM	141	OG	SER		58.072	-2.689	20.567	1.00 32.27	A
ATOM	142	C	SER		56.108		21.820	1.00 27.93	A
			SER		55.829			1.00 28.23	A
MOTA	143	0	254	20	023				

MOTA	144	N	GLY	A	21	55.191	-3.911	22.576	1.00 25.87	A
ATOM	145	CA	GLY		21	53.797		.22.222	1.00 23.78	A
ATOM	146	C	GLY		21	53.076	-2.732	22.598	1.00 23.94	A
ATOM	147	ō	GLY		21	53.638	-1.840	23.247	1.00 24.81	A
ATOM	148	N	GTN		22	51.821	-2.641	22.187	1.00 20.60	A
ATOM	149	CA.	GLN		22	51.033	-1.470	22.495	1.00 19.67	A
ATOM	150	CB	GLN		22	51.239	-0.400	21.415	1.00 19.28	A
ATOM	151	CG	GLN		22	50.584	0.943	21.736	1.00 18.12	A
MOTA	152	CD	GLN		22	50.732	1.971	20.613	1.00 18.84	A
ATOM	153		GLM		22	51.694	2.749	20.576	1.00 19.77	A
ATOM	154	NE2	GLN	A	22	49.777	1.968	19.688	1.00 16.83	A
MOTA	155	С	GLN	A	22	49.573	-1.873	22.566	1.00 18.66	A
MOTA	156	0	GLN	A	22	49.128	-2.747	21.826	1.00 18.45	A
MOTA	157	N	TYR	A	23	48.842	-1.257	23.484	1.00 17.25	A
MOTA	158	CA	TYR	A	23	47.423	-1.529	23.615	1.00 16.53	A
MOTA	159	CB	TYR	A	23	47.127	-2.497	24.752	1.00 14.51	A
ATOM	160	CG	TYR	A	23	45.674	-2.904	24.760	1.00 12.67	A
MOTA	161	CD1	TYR	A	23	45.251	-4.070	24.121	1.00 13.38	A
ATOM	162	CE1	TYR	A	23	43.904	-4.415	24.070	1.00 13.23	A
MOTA	163	CD2			23	44.713	-2.093	25.346	1.00 11.07	A A
MOTA	164		TYR		23	43.365	-2.425	25.299	1.00 12.99 1.00 13.72	A
ATOM	165	CZ	TYR		23	42.964	-3.583	24.664	1.00 13.72	A
ATOM	166	OH	TYR		23	41.624	-3.907	24.611 23.860	1.00 16.88	A
MOTA	167	С	TYR		23	46.694	-0.220 0.491	24.824	1.00 16.57	A
ATOM	168	0	TYR		23	46.975	0.085	22.969	1.00 16.16	A
MOTA	169	N	THR		24	45.757	1.311	23.038	1.00 16.43	A
MOTA	170	CA	THE		24	44.975 45.594	2.405	22.136	1.00 18.41	A
ATOM	171	CB	THE THE		24 24	45.581	1.954	20.771	1.00 17.20	A
ATOM	172	CG2			24	47.029	2.692	22.537	1.00 18.64	A
MOTA	173	C	THE		24	43.570	1.058	22.499	1.00 15.15	A
ATOM	174 175	0	THE		24	43.314	0.037	21.879	1.00 15.70	A
ATOM ATOM	176	N	HIS		25	42.667	1.993	22.754	1.00 15.66	A
ATOM	177	CA	HIS		25	41.320	1.924	22.210	1.00 15.79	A
ATOM	178	СВ	HIS		25	40.243	1.834	23.297	1.00 13.55	A
ATOM	179	CG	HIS		25	39.956	0.430	23.734	1.00 15.91	A
ATOM	180		HIS		25	40.688	-0.704	23.624	1.00 13.86	A
ATOM	181		HIS		25	38.790	0.071	24.374	1.00 15.91	A
ATOM	182		HIS		25	38.815	-1.222	24.639	1.00 14.38	A
ATOM	183	NEZ	HI	S A	25	39.956	-1.715	24.193	1.00 16.99	A
ATOM	184	C	HIS	S A	25	41.176	3.212	21.437	1.00 14.18	A
MOTA	185	0	HI	S A	25	41.677	4.241	21.865	1.00 13.52	A
ATOM	186	N	GLI	JA	26	40.510	3.150	20.292	1.00 14.81	A
MOTA	187	CA	GL/	JΑ	26	40.333	4.329	19.462	1.00 16.96	A
MOTA	188	CB		σA	26	41.132	4.188	18.164	1.00 16.34	A
MOTA	189	CG		UΑ	26	42.644	4.158	18.311	1.00 18.80	A A
ATOM	190	æ		UA	26	43.345	4.036	16.958	1.00 22.68 1.00 26.77	A
ATOM	191		L GL		26	42.744	4.456	15.946	1.00 20.46	A
MOTA	192		2 GL		26	44.490	3.539	16.901 19.101	1.00 20.40	A
MOTA	193	С		U A	26	38.875	4.543	18.996	1.00 17.22	A
MOTA	194	0		U A	26	38.104	3.597 5.802		1.00 18.91	A
MOTA	195	N		EA		38.503 37.150	6.135		1.00 19.32	A
ATOM	196			E A		36.290	6.546		1.00 20.19	A
MOTA	197			E A E A		34.834			1.00 23.33	A
MOTA	198		1 PH			34.024			1.00 22.07	A
MOTA MOTA	199 200		2 PH			34.289			1.00 23.24	A
ATOM	201		1 PH			32.692			1.00 26.16	A
ATOM	202		2 PH			32.954		18.587	1.00 25.99	A
ATOM	203			Œ A		32.155		18.592		A
ATOM	204			ŒA		37.260		17.522		A
ATOM	205			Œ A		37.733		17.871		A
MOTA	206			P A		36.831	7.052	16.288		A
ATOM	207			P P		36.901	8.060			A
MOTA	208			P F		35.910	9.203			A
ATOM	209			3P #		34.472				A
MOTA	210		1 AS	SP A	28	34.266		_		A
ATOM	211		2 A			33.552				A
MOTA	212			SP A		38.297				A
MOTA	213	3 0		SP 2		38.467				A A
MOTA	214			LY 1		39.292				A
ATOM	219			LY		40.658				A
MOTA	210			LY A		41.437				A
ATOM	21	7 0	G)	LY I	A 29	42.62	1 9.01	, T2.0T4		**

MOTA	218	N	ASP	A	30	40.797	8.922	17.098	1.00 16.92	A
ATOM	219	CA	ASP		30	41.511	9.438	18.254	1.00 16.83	A
ATOM	220	CB	ASP		30	40.816	10.678 11.864	18.796 17.888	1.00 18.99 1.00 21.09	A A
MOTA MOTA	221 222	CG OD1	ASP		30 30	40.988 42.145	12.177	17.538	1.00 22.94	A
ATOM	223	OD2			30	39.971	12.478	17.525	1.00 21.68	A
ATOM	224	C	ASP		30	41.656	8.392	19.345	1.00 17.25	A
ATOM	225	0	ASP	A	30	40.777	7.553	19.543	1.00 15.40	A.
MOTA	226	N	GLU		31	42.784	8.453	20.041	1.00 16.77	A A
ATOM	227	CA	GLU		31 31	43.111 44.620	7.514 7.607	21.107 21.392	1.00 18.43 1.00 20.90	A
MOTA MOTA	228 229	CB CG	GLU GLU		31	45.147	6.853	22.608	1.00 24.68	A
ATOM	230	CD	GLU		31	46.678	6.924	22.702	1.00 27.25	A
ATOM	231	OE1	GLŪ	A	31	47.258	7.931	22.239	1.00 26.93	A
ATOM	232		GLU		31	47.302	5.985	23.242	1.00 27.21 1.00 17.51	A A
ATOM	233	C	GLU		31 31	42.296 42.361	7.777 8.863	22.375 22.952	1.00 17.51	A
MOTA MOTA	234 235	N O	GLN		32	41.525	6.784	22.807	1.00 15.52	A
ATOM	236	CA	GLN		32	40.726	6.942	24.020	1.00 16.47	A
ATOM	237	CB	GLN		32	39.542	5.980	24.009	1.00 15.91	A
ATOM	238	CG	GLN		32	38.439	6.399	23.065	1.00 15.97	A A
ATOM	239	CD	GLN GLN		32 32	37.292 37.478	5.419 4.228	23.071 22.808	1.00 20.20 1.00 18.09	A
ATOM ATOM	240 241		GLN		32	36.091	5.912	23.374	1.00 20.57	A
ATOM	242	C	GLN		32	41.584	6.701	25.255	1.00 16.61	A
ATOM	243	0	GLN	A	32	41.448	7.387	26.272	1.00 15.51	A
MOTA	244	N	PHE		33	42.470	5.720	25.151 26.239	1.00 15.59 1.00 16.34	A A
ATOM	245	CA CB	PHE		33 33	43.370 42.583	5.389 4.854	27.443	1.00 17.21	A
MOTA MOTA	246 247	CG	PHE		33	41.951	3.502	27.222	1.00 16.68	A
ATOM	24B		PHE		33	42.686	2.333	27.406	1.00 15.57	A
ATOM	249		PHE		33	40.598	3.397	26.903	1.00 18.54	A
MOTA	250		PHE		33	42.083	1.076 2.147	27.288 26.782	1.00 16.34 1.00 17.35	A A
ATOM	251 252	CEZ	PHE		33 33	39.983 40.729	0.983	26.702	1.00 16.56	A
MOTA MOTA	253	C	PHE		33	44.363	4.343	25.776	1.00 16.66	A
ATOM	254	Ō	PHE		33	44.209	3.746	24.712	1.00 16.85	A
MOTA	255	N	TYR		34	45.398	4.139	26.572	1.00 16.03	A
MOTA	256	CA	TYR		34	46.377	3.125	26.264 25.621	1.00 16.93 1.00 16.33	A A
MOTA MOTA	257 258	CB CG	TYR		34 34	47.636 48.528	3.730 4.541	26.523	1.00 17.31	A
ATOM	259		TYR		34	49.519	3.930	27.291	1.00 17.48	A
ATOM	260		TYR		34	50.367	4,683	28.097	1.00 19.16	A
ATOM	261	CD2			34	48.404	5.928	26.586	1.00 17.68	A
MOTA	262	CE2			34	49.244 50.224	6.690 6.060	27.388 28.141	1.00 19.73 1.00 20.10	A A
MOTA MOTA	263 264	CZ OH	TYF		34 34	51.044	6.815	28.941	1.00 23.02	A
ATOM	265	c	TYF		34	46.692	2.473	27.588	1.00 17.88	A
MOTA	266	0	TYF	A S	34	46.429	3.042	28.646	1.00 21.13	A
MOTA	267	N	VAI		35	47.213	1.261	27.535	1.00 17.31 1.00 18.89	A A
MOTA	268	CA	VAI VAI		35 35	47.571 46.950	0.570 -0.848	28.749 28.804	1.00 19.12	A
MOTA MOTA	269 270	CB CG1	VAI		35	47.589	-1.660	29.912	1.00 17.56	A
ATOM	271		VAI		35	45.454	-0.742	29.048	1.00 19.75	A
MOTA	272	C	VAJ		35	49.084	0.478	28.786	1.00 18.84	A
MOTA	273	0		ιA	35	49.701	-0.050	27.877 29.830	1.00 16.51 1.00 22.55	A A
ATOM	274	N CA		PA PA	36 36	49.676 51.121	1.039 0.984	29.996	1.00 25.86	A
MOTA MOTA	275 276	CB		PA	36	51.542	1.872	31.172	1.00 26.89	A
ATOM	277	CG	AS	P A	36	53.033	2.108	31.221	1.00 26.55	A
MOTA	278		LAS		36	53.796	1.125	31.270	1.00 29.78	A
MOTA	279		AS	PA PA	36 36	53.441 51 393	3.285 -0.484	31.213 30.314	1.00 30.03 1.00 26.39	A A
MOTA MOTA	280 281	C		PA	36 36	51.393 51.016		31.378	1.00 27.38	A
ATOM	282	N		UA	37	52.024			1.00 27.51	A
MOTA	283	CA	LE	U A	37	52.305	-2.600		1.00 29.51	A
MOTA	284	CB		A U	37	52.754				A A
MOTA	285	CG	LE 1 LE	U A T D	37 37	51.704 52.265				A
MOTA MOTA	286 287		5 PE T PR			50.455				A
ATOM	288	C		UA		53.348				A
MOTA	289	0		U A		53.222				A
MOTA	290	N		YA		54.362				A A
MOTA	291	CA	GL	Y A	. 38	55.403	-2.140	31.737	1.00 35.44	A

ATOM	292	C	GLY		38	54.956	-1.863	33.162	1.00 37.63	A
ATOM	293	0	GLY		38	55.369	-2.549	34.098	1.00 38.42	A
MOTA	294	N	ARG		39	54.101	-0.861	33.334	1.00 38.93	A
ATOM	295	CA	ARG		39	53.625	-0.499	34.660	1.00 40.81	A
MOTA	296	CB	ARG		39	53.645	1.029	34.803	1.00 42.41	A A
MOTA	297	CG	ARG		39	54.968	1.627	34.339 34.619	1.00 44.76 1.00 47.83	A
ATOM	298	CD	ARG		39	55.113 56.318	3.118 3.644	33.976	1.00 50.52	A
ATOM	299	NE			39	56.902	4.799	34.281	1.00 53.40	A
ATOM	300	CZ	ARG		39 39	56.399	5.575	35.235	1.00 54.01	A
MOTA	301		ARG		39	57.998	5.179	33.633	1.00 54.18	A
ATOM ATOM	302 303	C	ARG		39	52.229	-1.057	34.936	1.00 41.12	A
ATOM	304	ō	ARG		39	51.664	-0.847	36.014	1.00 39.71	A
ATOM	305	N	LYS		40	51.687	-1.779	33.955	1.00 40.65	A
ATOM	306	CA	LYS		40	50.365	-2.380	34.070	1.00 39.55	A
ATOM	307	CB	LYS		40	50.415	-3.554	35.053	1.00 42.42	A
ATOM	308	CG	LYS	A	40	49.196	-4.467	34.996	1.00 46.46	A
ATOM	309	ÇD	LYS	A	40	49.266	-5.563	36.054	1.00 50.42	A
MOTA	310	CE	LYS	A	40	48.077	-6.513	35.947	1.00 51.25	A
MOTA	311	NZ	LYS		40	46.781	-5.779	35.970	1.00 52.15	A
ATOM	312	C	LYS		40	49.338	-1.348	34.540	1.00 37.45	A
MOTA	313	0	LYS		40	48.647	-1.560	35.533	1.00 35.78	A A
MOTA	314	N	GLU		41	49.245	-0.237	33.812	1.00 35.81 1.00 33.83	A
ATOM	315	CA	GLU		41	48.317	0.847	34.142 34.655	1.00 36.46	A
ATOM	316	CB	GLU		41 41	49.077 49.660	2.079 1.997	36.049	1.00 41.33	A
MOTA	317	CD CG	GLU		41	50.500	3.224	36.374	1.00 44.23	A
MOTA	318 319		GLU		41	50.067	4.343	36.022	1.00 46.67	A
MOTA MOTA	320	OE2			41	51.585	3.076	36.981	1.00 45.55	A
MOTA	321	C	GLU		41	47.492	1.301	32.937	1.00 30.89	A
ATOM	322	ō	GLU		41	47.995	1.373	31.816	1.00 27.89	A
ATOM	323	N	THE		42	46.227	1.623	33.182	1.00 28.11	A
ATOM	324	CA	THR	A	42	45.354	2.127	32.135	1.00 26.58	A
MOTA	325	CB	THE	A	42	43.882	1.773	32.406	1.00 27.67	A
ATOM	326	OG1	THE	A	42	43.716	0.349	32.394	1.00 25.55	A
MOTA	327	CG2	THE	A	42	42.979	2.419	31.357	1.00 25.33	A
MOTA	328	С	THE		42	45.506	3.642	32.212	1.00 26.90	A A
MOTA	329	0	THE		42	45.305	4.232	33.269	1.00 25.79 1.00 25.87	A
MOTA	330	N	VAI		43	45.881	4.273 5.720	31.108 31.106	1.00 24.36	A
ATOM	331	CA	VAI		43 43	46.045 47.474	6.119	30.670	1.00 24.45	A
ATOM	332	CB	VAI VAI		43	47.698	7.606	30.906	1.00 24.38	A
MOTA	333 334	CG2			43	48.504	5.289	31.433	1.00 22.82	A
MOTA MOTA	335	C		À	43	45.039	6.331	30.141	1.00 24.94	A
ATOM	336	ō		A	43	45.143	6.133	28.930	1.00 24.72	A
MOTA	337	N		P A	44	44.063	7.065	30.672	1.00 24.50	A
ATOM	338	CA		P A	44	43.050	7.681	29.824	1.00 25.64	A
ATOM	339	CB	TRI	P A	44	41.804	8.033	30.642	1.00 25.03	A
ATOM	340	CG	TRI	P A	44	41.224	6.859	31.370	1.00 25.96	A
MOTA	341	CD	2 TR		44	40.281	5.906	30.858	1.00 25.77	A
ATOM	342	CE:		PΑ	44	40.067	4.946	31.870	1.00 26.64	A
MOTA	343		3 TR			39.599	5.766	29.641	1.00 24.94	A A
MOTA	344		L TR			41.529	6.450	32.634 32.942	1.00 26.28	A
MOTA	345		1 TR			40.840 39.197	5.305 3.860	31.704	1.00 25.00	A
MOTA	346		2 TR 3 TR			38.734	4.688	29.476	1.00 22.40	A
ATOM	347 348		2 TR			38.542	3.749		1.00 24.18	A
ATOM ATOM	349			PΑ		43.578			1.00 26.30	A
ATOM	350			PΑ		44.321	9.713		1.00 24.42	A
ATOM	351			s A		43.193	9.090	27.853	1.00 28.01	A
ATOM	352			S A		43.635	10.234		1.00 30.22	A
ATOM	353		CX	SA	45	44.069	9.777		1.00 29.51	A
MOTA	354	SG	CY	SA	45	45.547				A
MOTA	355	С		SA		42.574				A
MOTA	356			SA		42.836				A
ATOM	357			UA		41.375				A A
MOTA	358			UA		40.261				A
MOTA	359			ע מ ע מ		39.137 38.810				A
MOTA	360		1 LE			37.492				A
ATOM	361 362		2 LE			38.710				A
MOTA MOTA	363			UF		39.734				A
ATOM	364			U I		39.195				A
MOTA	365			10 7		39.893			1.00 32.52	A

		-	~~~		45	40.488	14 442	28.986	1.00 32.23	A
ATOM	366		PRO PRO		47 47	39.437	14.442	30.901	1.00 32.23	A
ATOM ATOM	367 368		PRO		47	39.487	14.908	31.063	1.00 32.11	A
ATOM	369	CG	PRO		47	40.690	15.270	30.236	1.00 31.60	A
ATOM	370	c	PRO		47	38.066	12.800	31.245	1.00 30.96	A
ATOM	371	0	PRO		47	37.927	12.103	32.243	1.00 30.17	A
ATOM	372	N	VAL	A	48	37.064	13.068	30.418	1.00 30.75	A
ATOM	373	CA	VAL	A	48	35.715	12.563	30.663	1.00 32.56	A
ATOM	374	CB	VAL		48	34.748	13.040	29.560	1.00 34.04	A
MOTA	375	CG1			48	33.320	12.683	29.932	1.00 34.16	A
MOTA	376		VAL		48	34.881	14.556	29.368	1.00 38.02 1.00 33.13	A A
ATOM	377	C	VAL		48	35.633	11.033 10.485	30.765 31.355	1.00 33.15	A
ATOM	378	0	VAL		48 49	34.698 36.615	10.350	30.192	1.00 33.30	A
MOTA MOTA	379 380	N CA	LEU		49	36.661	8.892	30.208	1.00 32.44	A
ATOM	381	CB	LEU		49	37.498	8.391	29.023	1.00 30.62	A
ATOM	382	CG	LEU		49	36.792	8.027	27.702	1.00 31.64	A
	- 383	CD1			49	35.578	8.888	27.464	1.00 29.12	A
ATOM	384	CD2	LEU	Α	49	37.783	8.157	26.551	1.00 31.05	A
ATOM	385	C	LEU	A	49	37.226	8.343	31.519	1.00 33.77	A
MOTA	386	0	LEU		49	37.138	7.142	31.787	1.00 34.14	A
ATOM	387	N	ARG		50	37.794	9.221	32.339	1.00 34.56 1.00 35.58	A A
ATOM	388	CA	ARG		50	38.367	8.810 10.009	33.618 34.345	1.00 37.99	A
ATOM	389	CB	ARG		50 50	38.987 40.137	10.720	33.636	1.00 40.65	A
MOTA	390	CD	ARG		50	40.657	11.846	34.529	1.00 43.05	A
ATOM ATOM	391 392	NE	ARG		50	41.603	12.748	33.872	1.00 44.85	A
ATOM	393	CZ	ARG		50	42.815	12.403	33.444	1.00 46.08	A
ATOM	394		ARG		50	43.254	11.159	33.592	1.00 46.76	A
ATOM	395	NH2			50	43.599	13.314	32.880	1.00 46.08	A
MOTA	396	C	ARG	Α	50	37.334	8.168	34.547	1.00 35.55	A
MOTA	397	0	ARG	A	50	37.693	7.475	35.495	1.00 35.21	A
ATOM	398	N	GIT.	I A	51	36.054	8.412	34.284	1.00 36.77	A
MOTA	399	CA	GL1		51	34.987	7.859	35.116	1.00 37.34	A
ATOM	400	CB	GL4		51	33.658	8.558	34.821	1.00 39.02 1.00 41.24	A A
MOTA	401	CG	GLA		51	33.123	8.306 8.947	33.418 33.189	1.00 43.49	A
ATOM	402	CD	GF7 GF7		51 51	31.765 30.781	8.597	33.843	1.00 43.80	A
MOTA MOTA	403 404	NE2			51	31.706	9.895	32.260	1.00 44.01	A
ATOM	405	C	GL		51	34.821	6.362	34.896	1.00 36.85	A
ATOM	406	ō	GLI		51	34.250	5.665	35.734	1.00 37.06	A
MOTA	407	N	PHI	3 A	52	35.316	5.871	33.764	1.00 35.13	A
ATOM	408	CA	PHI	A	52	35.218	4.454	33.446	1.00 32.82	A
MOTA	409	СB	PHI		52	35.143	4.258	31.931	1.00 31.28	A
MOTA	410	CG	PHI		52	33.902	4.838	31.301	1.00 29.86	A A
MOTA	411		PHI		52	32.640	4.549	31.821 30.177	1.00 27.82 1.00 27.71	A
ATOM	412		PHI		52	33.992	5.652 5.060	31.234	1.00 25.58	A
MOTA	413	CE2	PHI		52 52	31.490 32.847	6.171	29.580	1.00 28.10	A
MOTA MOTA	414 415	CZ		ΕA	52	31.592	5.873	30.111	1.00 28.21	A
ATOM	416	C		ΕA	52	36.405	3.675	34.004	1.00 32.57	A
ATOM	417	ō		ΕA	52	37.370	4.256	34.494	1.00 32.22	A
MOTA	418	N		G A	53	36.327	2.353	33.927	1.00 32.80	A
ATOM	419	CA	AR	g A	53	37.397	1.498	34.419	1.00 32.77	A
ATOM	420	CB		g A		37.005	0.862	35.760	1.00 36.56	A
MOTA	421	CG		G A		36.741	1.867		1.00 42.83	A A
MOTA	422	CD		G A		36.523	1.168 2.111		1.00 49.04 1.00 53.82	A A
ATOM	423	NE		G A		36.308 36.195	1.758			A
MOTA	424	CZ	AR L AR	GA CA		36.277	0.478			A
MOTA	425 426		AR			36.004	2.683			A
ATOM ATOM	427	C		G A		37.706	0.404			A
MOTA	428	ō		G A		36.806	-0.117		1.00 28.71	A
ATOM	429			E A		38.986	0.066			A
ATOM	430			E A		39.440				A
MOTA	431		PH	e a	54	39.905				A
ATOM	432			E A		40.181		_		A
ATOM	433		l PH			39.150				A
ATOM	434		2 PH			41.471				A A
MOTA	435		1 PH			39.399				A
MOTA	436		2 PH	E A		41.733 40.697				A
MOTA MOTA	437 438			œ #		40.597				A
ATOM	439			E P		41.631				A
		-			- <b>-</b>					

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MOTA	440	N	ASP	A	55	40.408	-3.011	33.198	1.00 22.82	A
ATOM	441	CA	ASP	A	55	41.411	-3.874	33.805	1.00 24.70	A
ATOM	442	CB	ASP	A	55	40.785	-5.246	34.083	1.00 23.26	A
ATOM	443	CG	ASP		55	41.729	-6.190	34.789	1.00 26.24	A
								34.933	1.00 28.75	A
ATOM	444		ASP		55	42.924	-5.853			
ATOM	445	OD2	ASP	A	55	41.274	-7.279	35.192	1.00 26.38	A
ATOM	446	С	ASP	A	55	42.613	-4.011	32.861	1.00 24.24	A
ATOM	447	0	ASP	Α	55	42.510	-4.629	31.802	1.00 23.91	A
		N	PRO		56	43.770	-3.437	33.238	1.00 23.69	A
ATOM	448						-2.761	34.509	1.00 23.79	A
ATOM	449	Э	PRO		56	44.084				
MOTA	450	CA	PRO	A	56	44.961	-3.522	32.387	1,00 23.45	A
ATOM	451	CB	PRO	A	56	46.002	-2.707	33.162	1.00 23.35	A
ATOM	452	CG	PRO	A	56	45.592	-2.897	34.580	1.00 23.31	A
	453	C	PRO		56	45.413	-4.952	32.114	1.00 23.66	A
ATOM							-5.220	31.125	1.00 23.15	A
MOTA	454	0	PRO		56	46.099				A
MOTA	455	N	GLN	A	57	45.025	-5.871	32.991	1.00 21.84	
ATOM	456	CA	GLN	A	57	45.397	-7.261	32.818	1.00 22.47	A
ATOM	457	CB	GLN	A	57	44.834	-8.108	33.965	1.00 23.11	A
ATOM	458	CG	GLN		57	45.226	-9.568	33.873	1.00 20.82	A
					57	46.722	-9.745	33.733	1.00 22.23	A
MOTA	459	CD	GLN						1.00 21.88	A
MOTA	460	OE1	GLN	A	57	47.497	-9.227	34.539		
ATOM	461	NE2	GLN	A	57	47.138	-10.475	32.707	1.00 23.15	A
ATOM	462	C	GLN	A	57	44.882	-7.792	31.482	1.00 22.21	A
ATOM	463	o	GLN		57	45.452	-8.723	30.913	1.00 23.00	A
			PHE		58	43.801	-7.203	30.980	1.00 22.42	A
ATOM	464	N						29.704	1.00 21.07	A
ATOM	465	CA	PHE		58	43.254	-7.640			
ATOM	466	CB	PHE	A	58	42.004	-6.857	29.338	1.00 20.45	A
MOTA	467	CG	PHB	A	58	41.411	-7.287	28.031	1.00 21.03	A
ATOM	468	CD1	PHE	Α	58	40.472	-8.312	27.988	1.00 18.42	A
MOTA	469	CD2			58	41.864	-6.736	26.835	1.00 18.79	A
					58	39.992	-8.792	26.765	1.00 21.25	A
MOTA	470		PHE						1.00 20.28	A
ATOM	471		PHE		58	41.393	-7.207	25.610		
MOTA	472	$\mathbf{cz}$	PHE	Α	58	40.457	-8.238	25.578	1.00 21.18	A
ATOM	473	C	PHE	Α	58	44.278	-7.401	28.612	1.00 21.79	A
ATOM	474	ō	PHE		58	44.529	-8.260	27.763	1.00 21.84	A
			ALA		59	44.849	-6.202	28.637	1.00 21.80	A
MOTA	475	N							1.00 21.67	A
MOTA	476	CA	ALA		59	45.840	-5.801	27.657		
ATOM	477	CB	ALA	A	59	46.254	-4.346	27.892	1.00 21.11	A
ATOM	478	C	ALA	A	59	47.053	-6.711	27.732	1.00 22.06	A
ATOM	479	ō	ALA		59	47.518	-7.213	26.706	1.00 22.53	A
			LEU		60	47.561	-6.925	28.945	1.00 19.83	A
ATOM	480	N						29.116	1.00 20.88	A
MOTA	481	CA	LEU		60	48.729	-7.777			A
MOTA	482	CB	LEU	JA	60	49.163	-7.815	30.585	1.00 20.57	
ATOM	483	CG	LEU	JA	60	50.060	-6.657	31,053	1.00 24.17	A
ATOM	484	CD1	LEC	JA	60	49.239	-5.392	31.205	1.00 24.16	A
ATOM	485		LEU		60	50.717	-7.012	32.382	1.00 24.31	A
					60	48.496	-9.193	28.598	1.00 20.44	A
MOTA	486	C	LEC					27.955	1.00 21.97	A
MOTA	487	0	LEU		60	49.367	-9.770			
ATOM	488	N	THE	A S	61	47.319	-9.749	28.871	1.00 20.69	A
ATOM	489	CA	THE	A S	61	46.997	-11.101	28.418	1.00 19.49	A
ATOM	490	СВ	тнг	A S	61	45.697	-11.629	29.084	1.00 18.59	A
	491	OG			61		-11.830	30.489	1.00 21.12	A
MOTA							-12.942	28.453	1.00 17.61	A
MOTA	492		THE		61					A
MOTA	493	C		R S	61		-11.140	26.903	1.00 19.22	
MOTA	494	0	TH	RΣ	61		-12.059	26.242	1.00 21.19	A
MOTA	495	N	ASI	A	62	46.152	-10.142	26.351	1.00 18.05	A
ATOM	496	CA		A V	62	45.934	-10.092	24.910	1.00 19.26	A
	497	СВ		A V		45.020	-8.910	24.552	1.00 20.51	A
MOTA						43.835	-9.324	23.680	1.00 22.06	A
MOTA	498	CG		A V		43.033				A
ATOM	499		1 AS				-10.482	23.693	1.00 21.71	
ATOM	500	ND:	2 ASI	A n	62	43.294	-8.371	22.930	1.00 20.64	A
MOTA	501	C	AS	A N	62	47.270	-9.975	24.188	1.00 18.14	A
MOTA	502			N A			-10.681	23.217	1.00 19.73	A
				E A		48.146	-9.108	24.684	1.00 18.98	A
ATOM	503						-8.921	24.061	1.00 19.88	A
MOTA	504			EA		49.448				
ATOM	505	ÇB	IL	EΑ	. 63	50.229	-7.757	24.725	1.00 21.31	A
MOTA	506	CG	2 IL	E A	. 63	51.601	-7.590	24.064	1.00 20.11	A
ATOM	507		1 IL			49.425	-6.457	24.599	1.00 20.91	A
MOTA	508		1 IL			49.037		23.171	1.00 16.67	A
						En 247	-10.212		1.00 20.35	A
MOTA	509			E A		50.447	_10.520	22 202		A
MOTA	510			E A		51.048	-10.538	23.297	1.00 21.37	
MOTA	511	. <b>N</b>	AL	A A	64	50.028	-10.949	25.247	1.00 22.48	A
MOTA	512		AL	AA	64	50.713	-12.222	25.423	1.00 23.35	A
MOTA	513			AA		50.373	-12.816	26.785	1.00 22.29	A
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MOTA	514	C	ALA A		64	50.252 -		24.301	1.00 23.03	A
MOTA	515	0	ALA A		64	51.032 -		23.766	1.00 25.08 1.00 23.28	A A
ATOM	516 517	N CA	VAL I		65 65	48.976 -:		23.948 22.888	1.00 23.25	A
ATOM ATOM	518	CB	VAL 2		65	46.887 -		22.859	1.00 24.28	A
ATOM	519		VAL A		65	46.338 -		21.729	1.00 22.40	A
MOTA	520	CG2	VAL A	A	65	46.325 -		24.209	1.00 19.61	A
MOTA	521	C	VAL 1		65	49.013 -		21.538	1.00 23.88	A
ATOM	522	0	VAL 2		65	49.313 ~ 49.179 -		20.692 21.332	1.00 22.01 1.00 24.00	A A
ATOM ATOM	523 524	n Ca	LEU A		66 66	49.747 -		20.064	1.00 24.66	A
MOTA	525	CB	LEU J		66	49.872 -		20.011	1.00 22.13	A
ATOM	526	ÇG	LEU A		66	48.679	-9.228	20.117	1.00 23.81	A
MOTA	527	_	LEU 1		66		-8.001	19.277	1.00 20.24	A
ATOM	528		LEU I		66		-9.866	19.627	1.00 20.49 1.00 23.53	A A
ATOM ATOM	529	0	LEU I		66 66	51.143 - 51.548 -		19.906 18.813	1.00 22.08	A
ATOM	530 531	N	LYS		67	51.879 -		21.011	1.00 26.17	A
ATOM	532	CA	LYS		67	53.237 -		21.019	1.00 28.99	A
ATOM	533	СВ	LYS 2	A	67	53.839 -		22.421	1.00 29.27	A
ATOM	534	CG	LYS		67	55.278 -		22.548	1.00 30.64	A
MOTA	535	CD CD	LYS		67	55.779 - 57.159 -		23.976 24.157	1.00 32.41 1.00 35.25	A A
MOTA MOTA	536 537	CE NZ	LYS :		67 67	58.144 -		23.199	1.00 38.78	A
ATOM	538	C	LYS		67	53.200 -		20.598	1.00 29.87	A
ATOM	539	ō	LYS .		67	53.952 -	14.719	19.716	1.00 30.35	A
ATOM	540	N	HIS .		68	52.313 -		21.230	1.00 30.48	A
MOTA	541	CA	HIS .		68	52.163 -		20.922	1.00 31.95 1.00 34.42	A A
ATOM	542	CB	HIS.		68 68	51.051 - 50.827 -		21.775 21.520	1.00 38.63	A
ATOM ATOM	543 544	CDS	HIS		68 .	49.859 -		20.826	1.00 40.18	A
MOTA	545		HIS		68	51.676 -		21.992	1.00 41.00	A
ATOM	546		HIS		68	51.241 -		21.601	1.00 39.93	A
ATOM	547		HIS		68	50.141 -		20.891	1.00 39.69	A A
ATOM	548	C	HIS		68 68	51.828 - 52.463 -		19.448 18.746	1.00 31.53 1.00 32.07	A
ATOM ATOM	549 550	и О	HIS ASN		69	50.826 -		18.977	1.00 29.53	A
ATOM	551	CA	ASN		69	50.427 -		17.583	1.00 29.99	A
ATOM	552	CB	ASN		69	49.180 -		17.332	1.00 30.27	A
ATOM	553	CG	asn		69	47.918 -		17.885	1.00 31.83	A
MOTA	554		ASN		69	47.986 - 46.759 -		18.703 17.447	1.00 32.19 1.00 31.41	A A
ATOM	555 556	ND2	ASN ASN		69 69	51.552		16.638	1.00 30.37	A
MOTA MOTA	557	0	ASN		69	51.722		15.571	1.00 29.41	A
ATOM	558	N	LEU		70	52.324	-14.593	17.026	1.00 29.86	A
ATOM	559	CA	LEU		70	53.413		16.175	1.00 31.35	A
MOTA	560	СВ	LEU		70	54.039		16.751 15.950	1.00 28.55 1.00 28.77	A A
ATOM ATOM	561 562	CG	LEU LEU		70 70	55.190 · 54.745 ·		14.519	1.00 28.48	A
MOTA	563		LEU		70	55.651		16.627	1.00 27.89	A
ATOM	564	C	TEO		70	54.479		16.009	1.00 31.92	A
MOTA	565	0	LEU		70	54.994		14.914	1.00 31.72	A
ATOM	566	N	ASN		71	54.798 · 55.801 ·		17.097 17.060	1.00 34.09 1.00 38.27	A A
MOTA	567 568	CA CB	asn asn		71 71	55.884		18.427	1.00 39.70	A
MOTA MOTA	569	CG	ASN		71	56.490		19.490	1.00 44.05	A
ATOM	570		LASN		71	56.290	-16.955	20.693	1.00 44.98	A
MOTA	571		2 ASN		71	57.247		19.049	1.00 44.44	A
MOTA	572	C	ASN		71	55.484 56.358		15.983 15.224	1.00 38.32	. A
MOTA MOTA	573 574	N O	asn Ser		71 72	54.221		15.919	1.00 39.49	A
ATOM	575	CA	SER		72		-19.390	14.944	1.00 40.10	A
ATOM	576	СВ	SER		72	52.341	-19.816	15.256	1.00 41.05	A
MOTA	577	OG	SER		72		-20.763	14.311	1.00 42.44	A
MOTA	578	C	SER		72 72	53.860 54 336	-18.838 -19.516	13.523 12.608	1.00 40.66 1.00 40.90	A A
ATOM ATOM	579 580	N	Ser Leu		72 73		-17.608	13.341	1.00 39.86	A
ATOM	581	CA			73 73	53.408	-16.973	12.030	1.00 39.32	A
ATOM	582	CB			73	52.676	-15.632	12.082	1.00 38.99	A
MOTA	583	CG			73		-15.651	11.598	1.00 40.31	A
MOTA	584		l LEU		73 73		-16.860 -14.363	12.152 12.024	1.00 39.79 1.00 40.04	A A
atom Atom	585 586		TEO 5 TEO		73 73		-16.778	11.492	1.00 38.55	A
ATOM	587		LEU		73		-16.806	10.280	1.00 36.83	A

				_		FF 700	16 576	12 202	1.00 39.70	A
ATOM	588	N	ILE .		74	55.780 -		12.383		
ATOM	589	CA	ILE .	A	74	57.158		11.942	1.00 41.87	A
ATOM	590	CB	ILE .	A	74	58.104 -	-16.084	13.123	1.00 41.88	A
ATOM	591	CG2	ILE	A	74	59.552 ·	-16.054	12.640	1.00 41.29	A
ATOM	592		ILE		74	57.729	-14.734	13.738	1.00 41.53	A
ATOM	593		ILE		74	58.519		14.990	1.00 40.94	A
					74	57.599		11.273	1.00 42.04	A
ATOM	594	C	ILE					10.157	1.00 41.12	A
ATOM	595	0	ILE		74	58.119				
ATOM	596	N	LYS		75	57.364		11.954	1.00 43.51	A
ATOM	597	CA	LYS	A	75	57.730	-20.125	11.423	1.00 46.61	A
ATOM	598	CB	LYS	A	75	57.470	-21.217	12.466	1.00 47.84	A
ATOM	599	CG	LYS	A	75	58.096	-20.964	13.828	1.00 50.82	A
	600	CD	LYS		75	57.661		14.828	1.00 53.97	A
MOTA			LYS		75	58.005		16.269	1.00 55.95	· A
ATOM	601	CE				59.472		16.531	1.00 56.31	A
MOTA	602	ΝZ	LYS		75				1.00 47.99	A
ATOM	603	C	LYS	A	75	56.944		10.151		
MOTA	604	0	LYS	A	75	57.530		9.106	1.00 48.11	A
ATOM	605	N	ARG	A	76	55.617	-20.419	10.242	1.00 49.31	A
ATOM	606	CA	ARG	A	76	54.763	-20.742	9.103	1.00 50.89	A
	607	СВ	ARG		76		-20.744	9.530	1.00 53.08	A
ATOM			ARG		76		-21.847	10.538	1.00 56.83	A
ATOM	608	CG						10.574	1.00 58.85	A
ATOM	609	CD	ARG		76		-22.247		1.00 60.24	A
MOTA	610	NE	ARG	A	76		-21.253	11.212		
ATOM	611	$\mathbf{cz}$	ARG	A	76	49.786	-20.452	10.557	1.00 61.29	A
ATOM	612	NHl	ARG	A	76	49.692	-20.526	9.234	1.00 60.08	A
ATOM	613		ARG		76	49.044	-19.578	11.226	1.00 61.97	A
	614	С	ARG		76	54.947	-19.871	7.864	1.00 50.93	A
ATOM			ARG		76		-20.324	6.747	1.00 51.19	A
ATOM	615	0					-18.630	8.046	1.00 50.61	A
ATOM	616	N	SER		77				1.00 50.08	A
ATOM	617	CA	SER		77		-17.745	6.900		
ATOM	618	CB	SER	A	77		-16.295	7.282	1.00 50.05	Α.
ATOM	619	OG	SER	A	77	56.223	-15.787	8.193	1.00 49.23	A
ATOM	620	C	SER	A	77	57.006	-17.827	6.386	1.00 49.56	A
	621	ō	SER		77	57,420	-17.015	5.558	1.00 49.40	A
ATOM					78		-18.817	6.866	1.00 49.24	A
MOTA	622	N	ASN					6.472	1.00 49.14	A
MOTA	623	CA	ASN		78		-18.982		1.00 48.86	A
ATOM	624	CB	asn	A	78		-19.307	4.976		
MOTA	625	CG	ASN	Α	78		-19.689	4.558	1.00 48.09	A
ATOM	626	OD1	ASN	A	78	61.347	-20.442	5.254	1.00 46.05	A
ATOM	627	ND2	ASN	Α	78	61.109	-19.182	3.409	1.00 47.78	A
	628	c	ASN		78	59.857	-17.667	6.803	1.00 49.08	A
MOTA			ASN		78		-17.114	6.001	1.00 48.39	A
MOTA	629	0					-17.177	8.006	1.00 48.58	A
ATOM	630	N	SER		79			8.538	1.00 48.38	A
MOTA	631	CA	SER		79		-15.945			A
ATOM	632	CB	SER	Α	79		-16.208	9.071	1.00 48.53	
MOTA	633	OG	SER	A	79	62.415	-16.612	8.027	1.00 50.05	A
ATOM	634	C	SER	A	79	60.176	-14.768	7.573	1.00 47.13	A
ATOM	635	o	SER		79	61.197	-14.098	7.444	1.00 47.66	A
			THR		80		-14.516	6.887	1.00 45.82	A
MOTA	636	N					-13.379	5.982	1.00 45.51	A
ATOM	637	CA	THR		80			5.016	1.00 47.03	A
MOTA	638	CB	THR		80		-13.501			A
MOTA	639		l THR		80		-13.963	5.731	1.00 47.95	
MOTA	640	CG:	2 THE	ΑS	80		-14.487	3.909	1.00 47.59	A
ATOM	641	C	THE	A S	80	58.855	-12.147	6.882	1.00 44.25	A
ATOM	642		THE		80	57.835	-11.976	7.556	1.00 43.69	A
ATOM	643		ALA		81	59.889	-11.311	6.903	1.00 41.47	A
			ALZ				-10.119	7.740	1.00 38.59	A
MOTA	644					61.363		8.039	1.00 38.61	A
MOTA	645		AL						1.00 36.89	A
MOTA	646	C	ALI			59.168				A
MOTA	647	0	AL/	A A	81	58.766				
MOTA	648	N	AL	A A	82	58.993	-7.920			A
MOTA	649	CA	AL	A A	. 82	58.300	-6.690	7.698		A
ATOM	650			A A		57.957	-5.912	8.961	1.00 34.17	A
	651			AA		59.141				A
MOTA						60.372				A
ATOM	652			A A			_			A
MOTA	653			R A		58.457				A
MOTA	654	CA	. THI	R A	. 83	59.100				
MOTA	655	CB	TH	R A	83	58.377				A
ATOM	656		1 TH	R A	83	58.347	7 -5.562			A
ATOM	657		2 TH			59.098	_	2.578	1.00 34.35	A
MOTA	658			R A		59.04				A
						58.029				A
ATOM	659			R A						A
MOTA	660			N A		60.130				A
ATOM	663	L CA	AS	n P	84	60.18	8 -0.697	7 5.858	, 4.50 58.00	••

MOTA	662	CB	ASN	A	84	61.634	-0.252	6.069	1.00 36.13	A
ATOM	663	CG	asn	A	84	62.337	-1.045	7.132	1.00 37.22	A
MOTA	664		asn		84	61.809	-1.241	8.220	1.00 39.34	A
MOTA	665		ASN		84	63.548	-1.497	6.830	1.00 38.89	A A
ATOM	666	C	ASN		84	59.549	0.267 0.343	4.881	1.00 35.51 1.00 38.89	A
ATOM	667	И О	asn glu		84 85	59.961 58.546	1.004	5.344	1.00 34.17	A
ATOM ATOM	668 669	CA	GTA		85	57.890	2.001	4.507	1.00 32.82	A
ATOM	670	CB	GLU		85	56.427	2.183	4.921	1.00 36.55	A
ATOM	671	CG	GLU		85	55.523	0.993	4.645	1.00 42.74	A
MOTA	672	CD	GLU		85	55.271	0.782	3.167	1.00 46.65	A
MOTA	673	OE1	GLU	A	85	54.829	1.741	2.494	1.00 49.22	A
MOTA	674	OE2	GLU	A	85	55.508	-0.345	2.679	1.00 48.74	A
MOTA	675	C	GLU		85	58.624	3.328	4.701	1.00 30.10	A
MOTA	676	0	GLU		85	59.489	3.453	5.571	1.00 27.29 1.00 28.67	A A
ATOM	677	N	VAL		86	58.274 58.849	4.308 5.641	3.878 3.951	1.00 27.33	A
ATOM	678 679	CA CB	VAL VAL		86 86	59.146	6.202	2.539	1.00 27.74	A
ATOM ATOM	680		VAL		86	59.688	7.637	2.640	1.00 22.06	A
ATOM	681		VAL		86	60.139	5.289	1.815	1.00 25.30	A
ATOM	682	C	VAL		86	57.786	6.519	4.614	1.00 27.98	A
ATOM	683	0	VAL	A	86	56.685	6.671	4.086	1.00 28.76	A
ATOM	684	N	PRO	A	87	58.095	7.098	5.784	1.00 27.39	A
MOTA	685	CD	PRO		87	59.268	6.861	6.644	1.00 26.00	A
MOTA	686	CA	PRO		87	57.106	7.949	6.458	1.00 28.38	A.
MOTA	687	CB	PRO		B7	57.611	7.989	7.899 7.727	1.00 26.97 1.00 27.97	A A
ATOM	688	CG	PRO		87	59.099	7.915 9.341	5.848	1.00 30.15	A
MOTA	689	C	PRO PRO		87 87	56.963 57.902	9.871	5.245	1.00 31.62	A
MOTA MOTA	690 691	N O	GLU		88	55.778	9.922	6.004	1.00 29.70	A
ATOM	692	CA	GLU		88	55.489	11.252	5.481	1.00 29.65	A
ATOM	693	СВ	GLU		88	54.173	11.229	4.699	1.00 32.09	A
ATOM	694	CG	GLU		88	54.038	12.330	3.655	1.00 38.40	A
ATOM	695	СÐ	GLU	A	88	52.790	12.172	2.792	1.00 41.07	A
ATOM	696	OE1	GLU	A	88	51.675	12.411	3.303	1.00 42.35	A
ATOM	697	OE2			88	52.925	11.800	1.604	1.00 43.46	A
ATOM	698	C	GLU		88	55.385	12.191	6.680	1.00 27.98 1.00 26.16	A A
MOTA	699	0	GLU		88	54.588	11.954	7.597 6.672	1.00 28.16	A
ATOM	700	N	VAL		89	56.187 56.201	13.253 14.194	7.788	1.00 21.62	A
ATOM	701	CA CB	VAL VAL		89 89	57.637	14.358	8.333	1.00 18.36	A
ATOM ATOM	702 703		VAL VAL		89	57.639	15.295	9.534	1.00 17.11	A
ATOM	704		VAL		89	58.204	12.990	8.719	1.00 16.77	A
ATOM	705	C	VAL		89	55.626	15.575	7.483	1.00 21.60	A
MOTA	706	0	VAL	A	89	55.859	16.143	6.420	1.00 21.72	A
MOTA	707	N	THR	A	90	54.886	16.115	8.444	1.00 21.28	A
MOTA	708	CA	THR		90	54.269	17.425	8.301	1.00 20.62	A A
ATOM	709	CB	THR		90	52.813	17.303	7.823 6.613	1.00 21.90 1.00 26.43	A
ATOM	710		LTHR		90	52.770 52.220	16.537 18.678	7.558	1.00 23.70	A
ATOM ATOM	711 712	CG.	THR		90 90	54.264	18.153	9.639	1.00 21.08	A
ATOM	713	0	THE		90	53.887	17.578	10.667	1.00 20.41	A
ATOM	714	И	VAL		91	54.670	19.423	9.618	1.00 19.24	A
MOTA	715	CA	VAI		91	54.712	20.243	10.822	1.00 19.55	A
MOTA	716	CB	VAI	A	91	56.149	20.739	11.102	1.00 19.97	A
MOTA	717		l VAI		91	56.167	21.629	12.338	1.00 16.82	A
MOTA	718		2 VAI		91	57.072	19.547	11.280	1.00 17.43	A
MOTA	719	C	VAI		91	53.789	21.452	10.703	1.00 19.10 1.00 20.59	A A
ATOM	720	0	VAI			53.735 53.059	22.108 21.739	9.666 11.772	1.00 18.65	A
ATOM	721	N		A		52.146	22.870	11.785	1.00 19.10	A
MOTA MOTA	722 723	CA CB		A		50.853	22.516	11.030	1.00 18.89	A
ATOM	724	CG		3 A		50.176	21,264	11.525	1.00 16.16	A
ATOM	725		1 PH			49.165	21.331	12.480	1.00 16.77	A
ATOM	726		2 PHI			50.561	20.017	11.047	1.00 16.62	A
MOTA	727		1 PHI			48.543	20.168	12.955	1.00 18.06	A
MOTA	728		2 PHI			49.954		11.511	1.00 18.17	A
MOTA	729			BA		48.936		12.471	1.00 17.05	A A
ATOM	730			ΕA		51.844		13.229	1.00 19.48 1.00 19.64	A
ATOM	731			E A		52.055 51.365		14.134 13.445	1.00 19.64	A
MOTA MOTA	732 733			RA RA		51.365		14.792	1.00 19.26	A
ATOM	734			R A		51.275		14.921		A
ATOM	735			R A		50.435		14.043		A

3 = 0.14		-	amp			40 610	24 554	15 172	1.00 19.04	A
MOTA	736	C	SER		93	49.618	24.554	15.172		
ATOM	737	0	SER		93	48.748	24.417	14.316	1.00 17.44	A
ATOM	738	N	LYS	A	94	49.390	24.418	16.472	1.00 20.26	A
MOTA	739	CA	LYS	A	94	48.077	24.108	17.010	1.00 21.70	A
MOTA	740	CB	LYS	A	94	48.227	23.670	18.464	1.00 22.45	A
MOTA	741	CG	LYS	A	94	46.938	23.273	19.139	1.00 24.42	A
ATOM	742	CD	LYS		94	47.189	22.867	20.587	1.00 25.48	A
	743	CE	LYS		94	45.881	22.548	21.297	1.00 25.73	A
ATOM									1.00 26.34	A
ATOM	744	NZ	LYS		94	45.122	21.533	20.517		
ATOM	745	C	LYS		94	47.169	25.340	16.921	1.00 23.44	A
MOTA	746	0	LYS	A	94	45.984	25.235	16.598	1.00 20.95	A
MOTA	747	N	SER	A	95	47.742	26.505	17.212	1.00 24.82	A
ATOM	748	CA	SER	A	95	47.013	27.769	17.172	1.00 27.69	A
ATOM	749	CB	SER	A	95	46.969	28.408	18.565	1.00 26.33	A
ATOM	750	OG	SER		95	46.202	27.635	19.468	1.00 32.56	A
	751	C	SER		95	47.688	28.747	16.219	1.00 27.36	A
ATOM							28.529	15.797	1.00 27.94	A
MOTA	752	0	SER		95	48.824				
ATOM	753	N	PRO		96	46.985	29.830	15.849	1.00 27.27	A
ATOM	754	CD	PRO	A	96	45.611	30.232	16.193	1.00 28.85	A
ATOM	755	CA	PRO	A	96	47.606	30.801	14.946	1.00 26.90	A
ATOM	756	CB	PRO	Α	96	46.471	31.788	14.663	1.00 28.13	A
ATOM	757	CG	PRO	A	96	45.634	31.719	15.907	1.00 28.36	A
ATOM	758	C	PRO		96	48.786	31.421	15.700	1.00 24.92	A
		ō	PRO		96	48.757	31.556	16.925	1.00 24.65	A
ATOM	759								1.00 24.24	A
ATOM	760	N	VAL		97	49.828	31.786	14.973		
ATOM	761	CA	VAL		97	51.016	32.332	15.601	1.00 25.15	A
ATOM	762	CB	VAL		97	52.261	32.087	14.715	1.00 26.78	A
ATOM	763	CG1	VAL	A	97	53.531	32.372	15.508	1.00 26.15	A
ATOM	764	CG2	VAL	A	97	52.255	30.659	14.198	1.00 26.15	A
ATOM	765	C	VAL	Α	97	50.935	33.820	15.920	1.00 25.62	A
MOTA	766	0	VAL		97	50.624	34.638	15.054	1.00 25.01	A
	767	N	THR		98	51.207	34.157	17.175	1.00 24.46	A
ATOM								17.627	1.00 25.36	A
MOTA	768	CA	THR		98	51.212	35.542			
ATOM	769	CB	THR		98	49.835	35.941	18.283	1.00 25.29	A
ATOM	770	OG1	THR	A	98	50.030	37.008	19.217	1.00 30.50	A
MOTA	771	CG2	THR	A	98	49.196	34.771	18.985	1.00 29.80	A
ATOM	772	C	THR	A	98	52.382	35.678	18.605	1.00 24.87	A
ATOM	773	0	THR		98	52.499	34.902	19.554	1.00 23.01	A
ATOM	774	N	LEU		99	53.273	36.634	18.344	1.00 25.94	A
						54.445	36.843	19.198	1.00 28.02	A
ATOM	775	CA	LEU		99				1.00 31.12	A
MOTA	776	CB	LEU		99	55.194	38.114	18.797		
MOTA	777	CG	LEU		99	55.950	38.211	17.469	1.00 35.44	A
MOTA	778	CD1	LEU	A	99	56.650	39.577	17.416	1.00 35.45	A
MOTA	779	CD2	LEU	Α	99	56.970	37.087	17.341	1.00 35.62	A
ATOM	780	С	LEU	Α	99	54.135	36.932	20.689	1.00 27.10	A
MOTA	781	0	LEU	A	99	53.201	37.616	21.097	1.00 25.34	A
ATOM	782	N			100	54.935	36.233	21.492	1.00 26.71	A
		CA			100	54.762	36.253	22.935	1.00 26.48	A
ATOM	783				100		35.398	23.479	1.00 26.32	A
ATOM	784	C				53.635				A
ATOM	785	0			100	53.428	35.323	24.695	1.00 25.37	
ATOM	786	N	GLN	Α	101	52.913	34.734	22.585	1.00 25.16	A
MOTA	787	CA			101	51.796	33.896	22.999	1.00 25.74	A
MOTA	788	CB	GLN	Α	101	50.573	34.219	22.143	1.00 28.06	A
ATOM	789	CG	GLN	A	101	49.258	33.911	22.814	1.00 30.50	A
MOTA	790	æ	GLN	A	101	49.123	34.599	24.162	1.00 32.88	A
ATOM	791		GLN			48.953	35.820	24.251	1.00 30.83	A
	792		GLN			49.202	33.813	25.221	1.00 33.04	A
ATOM					101	52.117	32.409	22.901	1.00 24.01	A
MOTA	793	C							1.00 24.25	A
MOTA	794	0			101	52.280	31.881	21.807		
MOTA	795	N			102	52.199	31.715	24.051	1.00 22.08	A
MOTA	796	CD	PRC	) A	102	51.959	32.244	25.410	1.00 22.41	A
ATOM	797	CA	PRO	) A	102	52.500	30.278	24.096	1.00 21.37	A
ATOM	798	CB	PRO	A	102	52.136	29.898	25.526	1.00 21.61	A
ATOM	799	CG			102	52.521	31.147	26.297	1.00 21.90	A
ATOM	800	c			102	51.706	29.480	23.068	1.00 21.30	A
						50.496	29.644	22.947	1.00 21.93	A
MOTA	801	0			102				1.00 18.86	A
ATOM	802	N			103	52.396	28.618	22.327		A
MOTA	803	CA			103	51.749	27.802	21.305	1.00 17.69	
ATOM	804	CB			103	52.040	28.379		1.00 17.99	A
ATOM	805	CG	ASI	A I	103	50.899	28.162		1.00 18.28	A
ATOM	806	OD:	l asi	I A	103	50.348	27.060	18.808	1.00 17.82	A
ATOM	807				103	50.549	29.223		1.00 17.71	A
ATOM	808	C			103	52.281			1.00 15.57	A
MOTA	809	o			103	53.000			1.00 14.67	A
A Ou	009	9	wal							

ATOM	810	N	ILE A	104	51.918	25.565	20.397	1.00 15.80	A
MOTA	811	CA	ILE A	104	52.335	24.177	20.328	1.00 13.66	A
ATOM	812	CB	ILE A		51.255	23.235	20.888	1.00 15.40	A
	813		ILE A		51.589	21.792	20.539	1.00 13.82	A
ATOM									
MOTA	814		ILE A		51.132	23.421	22,400	1.00 17.40	A
MOTA	815	CD1	ILE A	104	50.129	22.494	23.047	1.00 18.65	A
ATOM	816	С	ILE A	104	52.588	23.775	18.896	1.00 14.36	A
ATOM	817	0	ILE A		51.716	23.924	18.052	1.00 16.86	A
								1.00 15.67	A
ATOM	818	N	LEU A		53.785	23.272	18.616		
ATOM	819	CA	LEU A	105	54.090	22.822	17.272	1.00 15.52	A
ATOM	820	CB	LEU A	105	55.568	22.978	16.940	1.00 15.73	A
ATOM	821	CG	LEU A	105	56.058	24.391	16.649	1.00 20.75	A
			LEU A		57.400	24.298	15.919	1.00 20.19	A
ATOM	822								A
ATOM	823		LEU A		55.030	25.141	15.791	1.00 21.31	
MOTA	824	С	LEU A	105	53.709	21.362	17.202	1.00 15.97	A
ATOM	825	0	LEU A	105	53.968	20.589	18.133	1.00 14.11	A
ATOM	826	N	ILE A	106	53.078	20.993	16.099	1.00 14.18	A.
			ILE A		52.643	19.630	15.903	1.00 15.40	A
MOTA	827	CA							
MOTA	828	CB	ILE A		51.122	19.576	15.636	1.00 15.11	A
MOTA	829	CG2	ILE A	106	50.661	18.135	15.592	1.00 12.46	A
ATOM	830	CG1	ILE A	106	50.380	20.354	16.734	1.00 15.51	A
ATOM	831		ILE A		48.862	20.413	16.565	1.00 12.83	A
							14.725	1.00 16.48	A
ATOM	832	C	ILE A		53.381	19.011			
ATOM	833	0	ILE A	106	53.484	19.607	13.651	1.00 17.37	A
ATOM	834	N	CYS A	107	53.900	17.811	14.944	1.00 17.86	A
ATOM	835	CA	CYS A	107	54.621	17.083	13.917	1.00 18.32	A
ATOM	836	C	CYS A		53.886	15.776	13.663	1.00 18.29	A
								1.00 18.13	A
ATOM	837	0	CYS A		53.846	14.909	14.533		
ATOM	838	CB	CYS A	107	56.041	16.792	14.382	1.00 19.33	A
ATOM	839	SG	CYS A	107	57.029	15.889	13.158	1.00 25.82	A
ATOM	840	N	LEU A	108	53.304	15.649	12.472	1.00 17.89	A
ATOM	841	CA	LEU A		52.556	14.456	12.088	1.00 18.82	A
							11.252	1.00 20.17	A
ATOM	842	CB.	LEU A		51.330	14.850			
ATOM	843	CG	LEU A	108	50.129	13.900	11.053	1.00 21.48	A
MOTA	844	CD1	LEU A	108	49.623	14.049	9.624	1.00 20.62	A
ATOM	845	CD2	LEU A	108	50.493	12.458	11.316	1.00 18.40	A
ATOM	846	C	LEU A		.53.445	13.538	11.252	1.00 19.49	A
					53.841	13.892	10.144	1.00 20.39	A
MOTA	847	0	LEU A						
MOTA	848	N	VAL A	109	53.760	12.368	11.789	1.00 18.45	A
MOTA	849	CA	VAL A	109	54.586	11.398	11.087	1.00 19.04	A
MOTA	850	CB	VAL A	109	55.665	10.805	12.042	1.00 18.71	A
MOTA	851		VAL A		56.626	9.923	11.279	1.00 15.16	A
						11.949	12.729	1.00 17.68	A
ATOM	852		VAL A		56.431				
ATOM	853	C	VAL A	. 109	53.611	10.322	10.606	1.00 20.50	A
ATOM	854	0	VAL A	109	53.115	9.516	11.393	1.00 21.55	A
ATOM	855	N	ASP A	110	53.326	10.337	9.308	1.00 21.50	A
ATOM	856	CA	ASP A	110	52.376	9.407	8.700	1.00 21.95	A
			ASP A		51.493	10.165	7.701	1.00 22.25	A
ATOM	857	CB							A
MOTA	858	CG	ASP A		50.084	9.612	7.622	1.00 24.20	
MOTA	859	ODI	. ASP A	110	49.874	8.435	7.989	1.00 23.87	A
ATOM	860	OD2	ASP A	110	49.182	10.356	7.182	1.00 25.94	A
ATOM	861	C	ASP A		53.059	8.240	7.985	1.00 21.53	A
			ASP A		54.273	8.254	7.782	1.00 18.80	A
MOTA	862	0				7.245	7.603	1.00 23.78	A
ATOM	863	N	ASN A		52.254				
ATOM	864	CA	asn a	111	52.706	6.037	6.900	1.00 23.32	A
MOTA	865	CB	asn a	111	53.046	6.360	5.437	1.00 24.67	A
ATOM	866	CG	ASN A	111	53.181	5.102	4.575	1.00 31.76	A
ATOM	867		ASN A		52.291	4.240	4.567	1.00 31.05	A
					54.292	4.994	3.842	1.00 29.09	A
MOTA	868		ASN A					1.00 23.68	
ATOM	869	C	asn A		53.905	5.389	7.587		A
MOTA	870	0	asn a	111	54.953	5.156	6.976	1.00 22.88	A
MOTA	871	N	ILE F	112	53.738	5.090	8.868	1.00 22.97	A
ATOM	872	CA	ILE A		54.797	4.473	9.646	1.00 20.73	A
		CB		1112	54.791	4.967	11.108	1.00 20.13	A
ATOM	873						11.864	1.00 15.53	A
ATOM	874		ITE 1		55.979	4.363			
MOTA	875		I ILE A		54.833	6.495	11.158	1.00 19.14	A
ATOM	876	CD:	l ILE A	112	54.671	7.058	12.575	1.00 20.42	A
ATOM	877			A 112	54.658	2.960	9.699	1.00 22.54	A
MOTA	878			A 112	53.605	2.436	10.054	1.00 22.65	A
					55.732	2.266	9.343	1.00 21.37	A
MOTA	879			A 113					A
MOTA	880			A 113	55.769	0.819			
MOTA	881	CB	PHE 2	A 113	54.742	0.167			A
MOTA	882		PHE 2	A 113	54.451	-1.252	8.850		A
ATOM	883		1 PHE		53.528	-1.543			A
VII	903	·	_ = = = = = = = =						

ATOM	884	CD2	PHE A 11	55.183	-2.296	8.285	1.00 20.76	A
ATOM	885	CEl	PHE A 11	53.341	-2.848	10.302	1.00 19.85	A
ATOM	886		PHE A 11		-3.607	8.721	1.00 20.75	A
ATOM	887	CZ	PHE A 11		-3.887	9.735	1.00 21.24	A
MOTA	888	C	PHE A 11		0.329	9.042	1.00 21.21	A A
MOTA	889	0	PHE A 11 PRO A 11		0.719 -0.509	8.011 9.893	1.00 19.97 1.00 22.22	A
ATOM ATOM	890 891	CD N	PRO A 11		-1.018	9.614	1.00 22.22	A.
ATOM	892	CA	PRO A 11		-1.040	11.170	1.00 23.38	A
ATOM	893	CB	PRO A 11		-2.045	11.571	1.00 23.68	A
ATOM	894	CG	PRO A 11		-1.435	10.984	1.00 23.26	A
ATOM	895	C	PRO A 11	4 57.078	0.059	12.221	1.00 24.33	A
ATOM	896	0	PRO A 11		1.174	12.054	1.00 24.35	A
ATOM	897	N	PRO A 11		-0.247	13.319	1.00 24.59	A
ATOM	898	CD	PRO A 11 PRO A 11		-1.472 0.751	13.567 14.372	1.00 22.60 1.00 23.79	A A
ATOM ATOM	899 900	CA CB	PRO A 11		0.751	15.107	1.00 23.96	A
MOTA	901	CG	PRO A 11		-1.291	14.998	1.00 23.45	A
ATOM	902	C	PRO A 11		0.996	15.289	1.00 24.97	A
ATOM	903	0	PRO A 11	5 57.322	0.670	16.482	1.00 23.11	A
ATOM	904	N	VAL A 11	6 58.380	1.573	14.705	1.00 24.77	A
MOTA	905	CA	VAL A 11		1.902	15.423	1.00 24.05	A
ATOM	906	CB	VAL A 11		0.881	15.135	1.00 26.45	A
ATOM	907		VAL A 11		1.250 -0.539	15.933 15.470	1.00 24.89 1.00 26.43	A A
MOTA	908 909	CG2	VAL A 11 VAL A 11		3.254	14.875	1.00 24.47	A
ATOM ATOM	910	o	VAL A 11		3.381	13.684	1.00 23.94	A
ATOM	911	N	VAL A 11		4.269	15.728	1.00 22.43	A
ATOM	912	CA	VAL A 11		5.577	15.239	1.00 22.18	A
ATOM	913	CB	VAL A 11	7 59.247	6.277	14.565	1.00 21.24	A
ATOM	914		VAL A 11		6.807	15.631	1.00 17.87	A
ATOM	915		VAL A 11		7.387	13.653	1.00 19.98 1.00 23.40	A A
ATOM	916	C	VAL A 11		6.484 6.323	16.326 17.512	1.00 23.40	A
ATOM	917	<b>И</b>	VAL A 11 ASN A 11		7.427	15.909	1.00 24.87	A
ATOM ATOM	918 919	CA	ASN A 11		8.398	16.833	1.00 25.96	A
ATOM	920	CB	ASN A 11		8.341	16.858	1.00 29.36	A
ATOM	921	CG	ASN A 11		7.213	17.728	1.00 31.24	A
MOTA	922	OD1	ASN A 13	8 63.885	6.833	18.722	1.00 34.20	A
MOTA	923		ASN A 11		6.694	17.374	1.00 34.04	A
MOTA	924	C	ASN A 11		9.746	16.312	1.00 24.87	A A
ATOM	925	0	ASN A 11		10.112 10.468	15.177 17.122	1.00 26.17 1.00 23.82	A
MOTA MOTA	926 927	N CA	ILE A 11		11.793	16.727	1.00 23.07	A
MOTA	928	СВ	ILE A 13		11.892	16.711	1.00 22.65	A
ATOM	929	CG2	ILE A 1	.9 58.797	13.197	16.051	1.00 18.01	A
MOTA	930		ILE A 1		10.716	15.936	1.00 21.02	A
MOTA	931		ILE A 1		10.714	15.921	1.00 21.88	A
MOTA	932	C	ILE A 1		12.771	17.754	1.00 22.76 1.00 22.92	A A
MOTA	933	0	THR A 1		12.680 13.691	18.940 17.303	1.00 22.32	A
ATOM ATOM	934 935	N CA	THR A 1		14.673	18.205	1.00 23.65	A
ATOM	936	CB	THR A 1		14.363	18.495	1.00 25.23	A
ATOM	937		THR A 1		14.199	17.258	1.00 26.55	A
MOTA	938	CG2	THR A 1	64.335	13.081	19.331	1.00 23.93	A
MOTA	939	C	THR A 1			17.616	1.00 23.20	A
ATOM	940	0	THR A 1			16.412	1.00 23.15 1.00 22.54	A
MOTA	941	N	TRP A 1:			18.470 17.998	1.00 21.37	A A
MOTA MOTA	942 943	CA CB	TRP A 1			18.791	1.00 19.43	. A
ATOM	944	CG	TRP A 1			18.616	1.00 18.76	A
ATOM	945		TRP A 1			17.703	1.00 19.96	A
ATOM	946		TRP A 1		18.454	17.931	1.00 18.06	A
ATOM	947		TRP A 1			16.715	1.00 16.07	A
ATOM	948		TRP A 1			19.330	1.00 18.18	A
ATOM	949		L TRP A 1			18.929	1.00 19.21 1.00 16.20	A A
MOTA	950		TRP A 1			17.210 16.000	1.00 16.43	A
MOTA MOTA	951 952		TRPA1			16.252	1.00 17.37	A
MOTA	953	C	TRP A 1				1.00 22.88	A
MOTA	954	ō	TRP A 1	21 64.743		18.992	1.00 22.75	A
MOTA	955	N	LEU A 1			17.164	1.00 23.24	A
MOTA	956	CA	LEU A 1				1.00 22.66	A
ATOM	957	CB	LEU A 1	22 66.094	20.699	15.850	1.00 23.05	A

N III OM	050	00	LEU A 122	66.638	19.293	15.563	1.00 22.23	A
ATOM	958	CG		67.404		14.253	1.00 20.93	A
ATOM	959		LEU A 122		19.326		1.00 20.21	A
MOTA	960		LEU A 122	67.542	18.830	16.700		
ATOM	961	C	LEU A 122	64.837	22.376	17.186	1.00 23.52	A
ATOM	962	0	LEU A 122	63.830	22.752	16.572	1.00 21.74	A
ATOM	963	N	SER A 123	65.579	23.174	17.945	1.00 23.69	A
ATOM	964	CA	SER A 123	65.330	24.597	18.063	1.00 24.10	A
ATOM	965	CB	SER A 123	64.998	24.983	19.504	1.00 25.22	A
MOTA	966	OG	SER A 123	64.735	26.373	19.591	1.00 25.55	A
ATOM	967	C	SER A 123	66.664	25.200	17.650	1.00 24.79	A
MOTA	968	0	SER A 123	67.670	25.014	18.335	1.00 23.07	A
ATOM	969	N	ASN A 124	66.666	25.903	16.521	1.00 25.02	A
ATOM	970	CA	ASN A 124	67.880	26.513	15.986	1.00 25.63	A
ATOM	971	CB	ASN A 124	68.351	27.676	16.868	1.00 24.46	A
ATOM	972	CG	ASN A 124	67.376	28.839	16.873	1.00 25.33	A
ATOM	973		ASN A 124	66.636	29.056	15.907	1.00 26.04	A
ATOM	974		ASN A 124	67.381	29.606	17.956	1.00 21.77	A
ATOM	975	C	ASN A 124	69.006	25.487	15.838	1.00 26.53	A
ATOM	976	ō	ASN A 124	70.132	25.706	16.301	1.00 26.36	A
MOTA	977	N	GLY A 125	68.684	24.361	15.205	1.00 24.78	A
	978	CA	GLY A 125	69.669	23.326	14.964	1.00 26.09	A
ATOM			GLY A 125	70.030	22.377	16.089	1.00 27.35	A
ATOM	979	C		70.728	21.395	15.846	1.00 28.21	A
ATOM	980	0	GLY A 125	69.566	22.645	17.307	1.00 28.65	A
MOTA	981	N	HIS A 126					A
ATOM	982	CA	HIS A 126	69.889	21.774	18.430	1.00 30.12 1.00 32.68	A
ATOM	983	CB	HIS A 126	70.816	22.507	19.408		
MOTA	984	CG	HIS A 126	70.226	23.750	19.996	1.00 35.25	A
ATOM	985		HIS A 126	70.296	25.044	19.601	1.00 36.90	A
MOTA	986		HIS A 126	69.475	23.743	21.151	1.00 35.93	A
ATOM	987	CE1	HIS A 126	69.110	24.979	21.445	1.00 36.88	A
ATOM	988	NE2	HIS A 126	69.595	25.788	20.520	1.00 36.73	A
MOTA	989	C	HIS A 126	68.661	21.220	19.149	1.00 30.87	A
MOTA	990	0	HIS A 126	67.634	21.889	19.270	1.00 31.49	A
MOTA	991	N	SER A 127	68.789	19.990	19.635	1.00 30.93	A
ATOM	992	CA	SER A 127	67.697	19.286	20.302	1.00 33.08	A
ATOM	993	СВ	SER A 127	68.165	17.889	20.714	1.00 33.91	A
ATOM	994	OG	SER A 127	69.231	17.979	21.645	1.00 38.34	A
ATOM	995	c	SER A 127	67.050	19.971	21.501	1.00 32.98	A
ATOM	996	ō	SER A 127	67.708	20.654	22.288	1.00 34.83	A
ATOM	997	N	VAL A 128	65.743	19.770	21.624	1.00 32.42	A
MOTA	998	CA	VAL A 128	64.960	20.325	22.716	1.00 31.29	A
		CB	VAL A 128	63.645	20.921	22.202	1.00 30.48	A
ATOM	999		VAL A 128	62.856	21.520	23.358	1.00 27.06	A
MOTA	1000		VAL A 128	63.937	21.970	21.142	1.00 28.52	A
MOTA	1001		VAL A 128		19.183	23.669	1.00 32.28	A
ATOM	1002	C	VAL A 128	64.645 64.275	18.093	23.237	1.00 32.80	A
MOTA	1003	0			19.437	24.965	1.00 33.30	A
MOTA	1004	N	THR A 129	64.786		25.981	1.00 33.70	A
MOTA	1005	CA	THR A 129	64.546	18.411		1.00 34.52	A
MOTA	1006	СВ	THR A 129	65.740	18.344	26.966	1.00 34.32	
ATOM	1007		THR A 129	65.969	19.643	27.528		A
MOTA	1008		THR A 129	67.006	17.898	26.245	1.00 34.60	A
ATOM	1009	C	THR A 129	63.257	18.591	26.791	1.00 32.08	A
ATOM	1010	0	THR A 129	62.645	17.615	27.220	1.00 34.04	A
ATOM	1011	N	<b>GLU A 130</b>	62.843	19.835	26.993	1.00 28.85	A
ATOM	1012	CA	GLU A 130	61.639	20.119	27.762	1.00 26.09	A
ATOM	1013	CB	GLU A 130	61.926	21.236	28.770	1.00 28.58	A
MOTA	1014	CG	<b>GLU A 130</b>	62.962	20.894	29.822	1.00 32.87	A
ATOM	1015	CD	GLU A 130	62.592	19.654	30.609	1.00 35.34	A
ATOM	1016	OEI	GLU A 130	61.392	19.475	30.907	1.00 37.85	A
ATOM	1017		GLU A 130	63.501	18.865	30.941	1.00 36.29	A
ATOM	1018	c	GLU A 130	60.451	20.534	26.893	1.00 23.53	A
MOTA	1019	ō	GLU A 130	60.629	21.166	25.859	1.00 19.76	A
		И	GLY A 131	59.243			1.00 21.13	A
MOTA	1020 1021	CA	GLY A 131	58.046		26.601	1.00 20.14	A
ATOM			GLY A 131	57.693			1.00 20.64	A
MOTA	1022	C	GLY A 131	56.989			1.00 20.11	A
ATOM	1023	0		58.989 58.164			1.00 18.28	A
MOTA	1024	N	VAL A 132				1.00 20.08	A
MOTA	1025	CA	VAL A 132	57.899			1.00 20.05	A
ATOM	1026	CB	VAL A 132	59.230			1.00 20.35	A
MOTA	1027		1 VAL A 132	58.946			1.00 22.11	
ATOM	1028		2 VAL A 132	60.006		_		A
ATOM	1029	C	VAL A 132	57.027				A
MOTA	1030	0	VAL A 132	57.194				A
MOTA	1031	N	SER A 133	56.094	15.948	23.925	1.00 17.90	A

ATOM	1032	CA	SER A 133	55.238	14.802	24.215	1.00 18.16	A
ATOM	1033	CB	SER A 133	54.045	15.206	25.094	1.00 18.24	A
ATOM	1034	OG	SER A 133	53.202	16.143	24.440	1.00 24.24	A
MOTA	1035	С	SER A 133	54.738	14.200	22.914	1.00 16.52	A
MOTA	1036	0	SER A 133	54.876	14.794	21.843	1.00 16.18	A
MOTA	1037	N	GLU A 134	54.166	13.009	22.996	1.00 17.45	A
ATOM	1038	CA	GLU A 134	53.653	12.369	21.800	1.00 18.50	A
ATOM	1039	CB	GLU A 134	54.797	11.661	21.050	1.00 22.31	A
ATOM	1040	CG	GLU A 134	55.475	10.513	21.801	1.00 24.62 1.00 28.65	A A
ATOM	1041	CD	GLU A 134	56.610	9.859 8.680	20.992 21.254	1.00 29.58	A
MOTA	1042		GLU A 134 GLU A 134	56.932 57.188	10.521	20.099	1.00 27.96	A
ATOM ATOM	1043 1044	C	GLU A 134	52.523	11.389	22.087	1.00 18.44	A
ATOM	1045	ŏ	GLU A 134	52.279	11.003	23.234	1.00 17.30	A
ATOM	1046	N	THR A 135	51.824	11.008	21.027	1.00 16.71	A
ATOM	1047	CA	THR A 135	50.733	10.059	21.119	1.00 15.49	A
ATOM	1048	CB	THR A 135	49.738	10.246	19.967	1.00 16.16	A
MOTA	1049	OG1	THR A 135	50.369	9.867	18.731	1.00 16.02	A
ATOM	1050	CG2		49.280	11.697	19.879	1.00 14.19	A
MOTA	1051	C	THR A 135	51.346	8.682	20.946	1.00 17.19	A
ATOM	1052	0	THR A 135	52.551	8.554	20.733	1.00 17.26	A
ATOM	1053	N	SER A 136	50.519	7.650	21.047	1.00 17.53 1.00 15.92	A A
ATOM	1054	CA	SER A 136	51.001	6.297 5.266	20.818 21.416	1.00 15.92	A
MOTA	1055	CB	SER A 136	50.035 49.756	5.532	22.781	1.00 18.22	A
ATOM	1056 1057	OG C	SER A 136 SER A 136	50.967	6.187	19.294	1.00 15.84	A
ATOM ATOM	1057	o	SER A 136	50.715	7.169	18.596	1.00 17.25	A
ATOM	1059	N	PHE A 137	51.236	5.003	18.767	1.00 17.08	A
ATOM	1060	CA	PHE A 137	51.155	4.806	17.333	1.00 15.67	A
ATOM	1061	CB	PHE A 137	51.874	3.519	16.936	1.00 13.47	A
MOTA	1062	CG	PHE A 137	53.363	3.628	16.951	1.00 14.48	A
MOTA	1063	CD1	PHE A 137	54.037	4.255	15.907	1.00 15.82	A
ATOM	1064		PHE A 137	54.100	3.112	18.010	1.00 15.21	A
ATOM	1065		PHE A 137	55.427	4.367	15.918	1.00 15.72	A
ATOM	1066	CE2		55.490	3.220	18.031	1.00 15.14 1.00 14.35	A A
ATOM	1067	CZ	PHE A 137	56.152	3.848 4.657	16.983 17.067	1.00 14.35	A
ATOM	1068	C	PHE A 137 PHE A 137	49.659 49.037	3.767	17.622	1.00 18.05	A
ATOM ATOM	1069 1070	N O	LEU A 138	49.074	5.534	16.259	1.00 17.51	A
ATOM	1071	CA	LEU A 138	47.648	5.433	15.953	1.00 19.20	A
ATOM	1072	СВ	LEU A 138	47.017	6.822	15.800	1.00 20.80	A
ATOM	1073	CG	LEU A 138	46.809	7.688	17.044	1.00 23.47	A
MOTA	1074	CD1	LEU A 138	46.141	6.879	18.144	1.00 24.75	A
MOTA	1075		LEU A 138	48.140	8.212	17.529	1.00 27.62	A
ATOM	1076	C	LEU A 138	47.490	4.637	14.658	1.00 18.41 1.00 16.16	A A
MOTA	1077	0	LEU A 138	48.218	4.862	13.698 14.630	1.00 18.51	A
MOTA	1078	N	SER A 139 SER A 139	46.530 46.333	3.716 2.863	13.460	1.00 17.61	A
MOTA MOTA	1079 1080	CA CB	SER A 139	45.481	1.656	13.836	1.00 18.17	A
ATOM	1081	OG	SER A 139	44.134	2.036	14.040	1.00 20.80	A
ATOM	1082	c	SER A 139	45.729	3.510	12.216	1.00 17.44	A
MOTA	1083	0	SER A 139	45.122	4.578	12.276	1.00 16.41	A
ATOM	1084	N	LYS A 140	45.908	2.822	11.088	1.00 18.56	A
ATOM	1085	CA	LYS A 140	45.402	3.237	9.778	1.00 18.37	A
ATOM	1086	CB	LYS A 140	46.543	3.751	8.895	1.00 21.60	A
ATOM	1087	CG	LYS A 140	47.149	5.085	9.326	1.00 24.86	A
MOTA	1088	CD	LYS A 140	46.513	6.267	8.602 7.150	1.00 30.27 1.00 29.93	A A
ATOM	1089	CE	LYS A 140	46.961 48.440	6.345 6.349	7.038	1.00 30.14	A
MOTA	1090	ΝZ	LYS A 140 LYS A 140	44.773	2.012	9.118	1.00 17.79	A
MOTA MOTA	1091 1092	Ö	LYS A 140	45.106	0.878	9.458	1.00 17.76	A
ATOM	1093	N	SER A 141	43.882	2.234	8.160	1.00 18.54	A
ATOM	1094	CA	SER A 141	43.220	1.124	7.481	1.00 21.55	A
ATOM	1095	CB	SER A 141	42.047	1.634	6.630	1.00 21.05	A
ATOM	1096	OG	SER A 141	42.490		5.588		A
MOTA	1097	C	SER A 141	44.154	0.263	6.625		A
MOTA	1098	0	SER A 141	43.828		6.332	1.00 21.49	A
MOTA	1099	N	ASP A 142	45.311		6.226		A A
MOTA	1100	CA	ASP A 142	46.234		5.430 4.420		A
MOTA	1101	CB	ASP A 142 ASP A 142	47.008 47.949		5.076		A
ATOM ATOM	1102 1103	CG.	ASP A 142 1 ASP A 142	47.949				A
ATOM	1103		2 ASP A 142	48.799				A
MOTA	1105	C	ASP A 142	47.176			1.00 20.11	A

ATOM	1106	0	ASP A 142	48.127	-1.416	5.946	1.00 19.21	A
MOTA	1107	N	HIS A 143	46.885	-0.626	7.659	1.00 18.99	A A
MOTA	1108	CA	HIS A 143	47.637 47.686	-1.295 -2.792	8.706 8.409	1.00 17.27 1.00 16.45	A
ATOM ATOM	1109 1110	CB CG	HIS A 143 HIS A 143	46.329	-3.396	8.190	1.00 18.33	A
ATOM	1111		HIS A 143	45.860	-4.211	7.213	1.00 17.59	A
ATOM	1112		HIS A 143	45.262	-3.151	9.032	1.00 15.97	A
MOTA	1113	CE1	HIS A 143	44.194	-3.786	8.580	1.00 19.46	A
MOTA	1114		HIS A 143	44.529	-4.436	7.478	1.00 18.06	A A
ATOM	1115	C	HIS A 143	49.019 49.812	-0.749 -1.401	9.030 9.715	1.00 19.46 1.00 19.95	A
MOTA MOTA	1116 1117	o N	HIS A 143 SER A 144	49.301	0.454	8.536	1.00 19.70	A
ATOM	1118	CA	SER A 144	50.542	1.141	8.852	1.00 20.18	A
ATOM	1119	CB	SER A 144	51.018	2.011	7.678	1.00 19.91	A
MOTA	1120	OG	SER A 144	50.099	3.044	7.364	1.00 23.64	A
ATOM	1121	C	SER A 144	50.109	2.018	10.034	1.00 19.40 1.00 19.70	A A
ATOM	1122	0	SER A 144	48.970	1.906 2.883	10.499 10.525	1.00 16.99	A
MOTA	1123	N CA	PHE A 145 PHE A 145	50.986 50.614	3.728	11.649	1.00 16.06	A
MOTA MOTA	1124 1125	CB	PHE A 145	51.325	3.274	12.929	1.00 16.25	A
ATOM	1126	CG	PHE A 145	51.062	1.841	13.297	1.00 19.53	A
ATOM	1127	CD1	PHE A 145	51.754	0.807	12.672	1.00 20.17	A
ATOM	1128		PHE A 145	50.114	1.522	14.263	1.00 18.18	A
MOTA	1129		PHE A 145	51.505	-0.525 0.193	13.005 14.606	1.00 21.33 1.00 19.50	A A
ATOM	1130	CE2	PHE A 145 PHE A 145	49.856 50.553	-0.831		1.00 20.23	A
MOTA MOTA	1131 1132	CZ C	PHE A 145	50.955	5.182	11.419	1.00 15.69	A
ATOM	1133	ŏ	PHE A 145	51.548	5.538	10.404	1.00 16.69	A
MOTA	1134	N	PHE A 146	50.530	6.021	12.357	1.00 14.53	A
MOTA	1135	CA	PHE A 146	50.869	7.429	12.332	1.00 16.67	A A
MOTA	1136	CB	PHE A 146	49.841	8.279 8.528	11.552 12.259	1.00 16.59 1.00 15.25	A
ATOM	1137	CG	PHE A 146 PHE A 146	48.535 48.370	9.644	13.071	1.00 15.42	A
MOTA MOTA	1138 1139		PHE A 146	47.433	7.708	12.019	1.00 16.06	A
MOTA	1140		PHE A 146	47.123	9.952	13.629	1.00 17.50	A
ATOM	1141	CE2	PHE A 146	46.180	8.003	12.571	1.00 16.80	A
MOTA	1142	CZ	PHE A 146	46.023	9.126	13.375	1.00 17.47 1.00 17.00	A A
ATOM	1143	C	PHE A 146	51.017 50.345	7.841 7.308	13.783 14.661	1.00 17.00	A
ATOM	1144 1145	O N	PHE A 146 LYS A 147	51.950	8.747	14.032	1.00 17.82	A
ATOM ATOM	1145	CA	LYS A 147	52.224	9.221	15.377	1.00 18.67	A
ATOM	1147	CB	LYS A 147	53.540	8.604	15.863	1.00 20.48	A
MOTA	1148	CG	LYS A 147	53.771	8.668	17.359	1.00 25.54	A
MOTA	1149	CD	LYS A 147	54.822	7.645	17.774	1.00 29.96 1.00 30.05	A A
ATOM	1150	CE	LYS A 147 LYS A 147	54.835 55.740	7.417 6.291	19.282 19.643	1.00 33.05	A
MOTA	1151 1152	NZ C	LYS A 147	52.315	10.743	15.338	1.00 17.25	A
MOTA MOTA	1152	Ö	LYS A 147	52.716	11.320	14.329	1.00 19.15	A
ATOM	1154	N	ILE A 148	51.932	11.391	16.428	1.00 15.47	A
MOTA	1155	CA	ILE A 148	51.969	12.846	16.494	1.00 14.99	A
MOTA	1156	CB	ILE A 148	50.529	13.424	16.642	1.00 15.37	A A
MOTA	1157		2 ILE A 148	50.566 49.689	14.932 13.025	16.740 15.426	1.00 14.06 1.00 16.41	A
MOTA	1158 1159		1 ILE A 148 1 ILE A 148	48.223	13.325	15.550	1.00 18.61	A
MOTA MOTA	1160	c.	ILE A 148	52.829	13.271	17.682	1.00 17.07	A
ATOM	1161	ō	ILE A 148	52.721	12.702	18.772	1.00 15.61	A
ATOM	1162	N	SER A 149	53.696	14.255	17.458	1.00 16.79	A
MOTA	1163	CA		54.570	14.757	18.514	1.00 17.66 1.00 15.95	A A
MOTA	1164	CB		56.042	14.612 14.956	18.116 19.190		A
MOTA	1165 1166		SER A 149 SER A 149	56.900 54.239	16.225	18.763		A
MOTA MOTA	1167		SER A 149	53.854	16.949	17.842		A
MOTA	1168		TYR A 150	54.401	16.665	20.005		A
ATOM	1169	CA	TYR A 150	54.085		20.362		A
MOTA	1170			52.893		21.310		A A
ATOM	1171			51.679		20.797 19.789		A
MOTA	1172		1 TYR A 150	50.879 49.733		19.769		A
MOTA MOTA	1173 1174		2 TYR A 150	51.313				A
ATOM	1175		2 TYR A 150	50.176		20.901		A
MOTA	1176			49.391	15.957			A
MOTA	1177			48.275				A A
ATOM	1178		TYR A 150	55.237				A
MOTA	1179	0	TYR A 150	55.953	18.207	24.04	2.00 25.05	•

MOTA	1180	N	LEU A	151	55.409	20.029	20.649	1.00 17.01	A
MOTA	1181	CA	LEU A		56.449	20.868	21.224	1.00 15.24	A
ATOM	1182	СВ	LEU A		57.540	21.182	20.197	1.00 16.33	A
MOTA	1183	CG	LEU A		58.487	22.335	20.575	1.00 16.27	A
ATOM ATOM	1184 1185		LEU A		59.402 59.315	21.906 22.755	21.706 19.359	1.00 17.13 1.00 19.34	A A
ATOM	1186	C	LEU A		55.825	22.174	21.666	1.00 16.08	A
ATOM	1187	õ	LEU A		55.221	22.881	20.860	1.00 16.22	A
ATOM	1188	N	THR A		55.952	22.497	22.945	1.00 16.84	A
ATOM	1189	CA	THR A	152	55.428	23.765	23.424	1.00 18.70	A
ATOM	1190	CB	THR A	152	55.283	23.799	24.946	1.00 20.14	A
MOTA	1191		THR A		56.576	23.633	25.544	1.00 23.32	A
MOTA	1192		THR A		54.355	22.694	25.419	1.00 18.36	A
ATOM	1193	C	THR A		56.498	24.772	23.050	1.00 20.04	A A
ATOM ATOM	1194	O N	THR A		57.689 56.085	24.448 25.986	23.034 22.735	1.00 20.72 1.00 20.63	A
ATOM	1195 1196	CA	LEU A		57.043	27.014	22.389	1.00 24.69	A
ATOM	1197	CB	LEU A		57.579	26.794	20.960	1.00 24.19	A
ATOM	1198	CG	LEU A		56.716	26.942	19.694	1.00 26.72	A
MOTA	1199	CD1	LEU A	153	55.303	26.451	19.959	1.00 27.32	A
ATOM	1200	CD2	LEU A	153	56.686	28.393	19.249	1.00 26.15	A
MOTA	1201	C	LEU A		56.410	28.385	22.531	1.00 26.36	A
ATOM	1202	0	LEU A		55.180	28.511	22.597	1.00 29.59	A
MOTA	1203	N	LEU A		57.262	29.401	22.620	1.00 26.29 1.00 26.89	A A
MOTA MOTA	1204 1205	CA CB	LEU A		56.830 57.459	30.787 31.444	22.729 23.965	1.00 26.89	A
ATOM	1205	CG	LEU A		56.966	32.833	24.407	1.00 28.58	A
ATOM	1207		LEU A		55.507	32.755	24.864	1.00 24.43	A
ATOM	1208		LEU A		57.845	33.342	25.549	1.00 27.14	A
MOTA	1209	C	LEU A	154	57.337	31.458	21.456	1.00 28.94	A
MOTA	1210	0	LEU A	. 154	58.538	31.689	21.304	1.00 30.73	A
MOTA	1211	N	PRO A		56.428	31.773	20.518	1.00 30.57	A
MOTA	1212	CD	PRO A		54.975	31.534	20.559	1.00 29.60	A
ATOM	1213	CA CB	PRO A		56.806 55.460	32.412 32.668	19.254 18.581	1.00 31.63 1.00 30.63	A A
MOTA MOTA	1214 1215	CG	PRO A		54.612	31.552	19.087	1.00 28.73	A
MOTA	1216	C	PRO A		57.639	33.688	19.370	1.00 33.58	A
MOTA	1217	0	PRO A		57.322	34.593	20.136	1.00 33.98	A
MOTA	1218	N	SER A	. 156	58.706	33.741	18.586	1.00 35.79	A
MOTA	1219	CA	SER A		59.595	34.888	18.546	1.00 37.77	A
MOTA	1220	CB	SER A		60.604	34.839	19.694	1.00 38.66	A
ATOM	1221	OG	SER A		59.955 60.332	34.966 34.841	20.949 17.222	1.00 44.00 1.00 38.83	A A
MOTA MOTA	1222 1223	C 0	SER A		60.352	33.849	16.492	1.00 38.36	A
ATOM	1224	N	ALA A		61.042	35.915	16.909	1.00 40.38	A
ATOM	1225	CA	ALA A		61.796	35.972	15.670	1.00 39.93	A
ATOM	1226	CB	ALA A	157	61.822	37.401	15.148	1.00 40.36	A
ATOM	1227	C	ALA A		63.214	35.466	15.918	1.00 39.65	A
MOTA	1228	0	ALA A		64.05B	35.504	15.021	1.00 39.72	A
MOTA	1229	N	GLU A		63.463	34.984	17.135 17.517	1.00 39.12	A A
MOTA	1230 1231	CA CB	GLU A		64.784 65.082	34.480 34.808	18.988	1.00 40.24 1.00 44.21	A A
ATOM ATOM	1232	CG	GLU A		65.426	36.268	19.287	1.00 50.31	A
ATOM	1233	CD	GLU Z		64.204	37.174	19.356	1.00 55.36	A
ATOM	1234		GLU I		64.353	38.351	19.765	1.00 55.75	A
ATOM	1235	OE2	GLU 2	158	63.095	36.712	19.002	1.00 58.12	A
MOTA	1236	C	GLU A		65.005	32.979	17.303	1.00 38.02	A
MOTA	1237	0	GLU A		66.130	32.493	17.419	1.00 36.30	A
MOTA	1238	N	GLU A		63.950	32.234	17.002 16.805	1.00 35.79 1.00 35.02	A A
ATOM ATOM	1239 1240	CA CB	GLU A		64.136 63.949	30.807 30.066	18.135	1.00 36.97	A
ATOM	1241	CG	GLU 1		62.699	30.439	18.891	1.00 41.68	A
ATOM	1242	æ	GLU A		62.717	29.933	20.323	1.00 44.82	A
ATOM	1243	OE1	GLU 2	A 159	62.819	28.705	20.527	1.00 46.62	A
MOTA	1244		GLU 1		62.631	30.767	21.248	1.00 47.25	A
MOTA	1245	C	GLU 2		63.277	30.162	15.735	1.00 32.21	A
MOTA	1246	0	GLU I		62.147	30.574	15.473	1.00 32.05	A N
ATOM	1247 1248	n Ca	SER A	A 160 A 160	63.849 63.167	29.147 28.394	15.107 14.076	1.00 29.55 1.00 28.89	A A
MOTA MOTA	1248	CB		4 160 4 160	63.885	28.551	12.734	1.00 27.34	A
ATOM	1250	OG		A 160	65.206	28.053	12.807	1.00 29.49	A
ATOM	1251	c		A 160	63.241	26.957	14.565	1.00 27.42	A
MOTA	1252	0	SER 2	A 160	64.092	26.628	15.392	1.00 25.45	A
MOTA	1253	N	TYR I	A 161	62.359	26.101	14.066	1.00 24.73	A

ATOM	1254	CA	TYR	A	161	62.359	24.725	14.517	1.00	24.26	A
MOTA	1255	CB	TYR	A	161	61.172	24.480	15.451	1.00	23.50	A
ATOM	1256	CG	TYR			60.935	25.593	16.434		24.01	A
MOTA	1257		TYR			60.255	26.748	16.052		26.02	A
ATOM	1258		TYR			60.009	27.774	16.959	1.00	27.93	A
MOTA	1259	CD2	TYR	Ą	161	61.374	25.491	17.753	1.00	24.78	A
ATOM	1260	CE2	TYR	A	161	61.136	26.514	18.674	1.00	25.93	A
ATOM	1261	CZ	TYR			60.450	27,650	18.270		27.56	A
ATOM	1262	OH	TYR			60.182	28.650	19.173		29.78	A
ATOM	1263	C	TYR			62.330	23.700	13.397	1.00	25.15	A
ATOM	1264	0	TYR	A	161	62.082	24.021	12.239	1.00	24.96	A
ATOM	1265	N	ASP	A	162	62.600	22.455	13.775	1.00	26,26	A
ATOM	1266	CA	ASP			62.598	21.331	12.858		26.94	A
		CB	ASP								
ATOM	1267					64.007	21.014	12.356		30.11	A
ATOM	1268	CĢ	ASP			64.548	22.067	11.434	1.00	32.85	A
MOTA	1269	OD1	ASP	A	162	64.075	22.138	10.277	1.00	33.31	A
ATOM	1270	OD2	ASP	Α	162	65.443	22.819	11.874	1.00	33.08	A
MOTA	1271	C	ASP	A	162	62.122	20.117	13.613	1.00	25.87	A
MOTA	1272	ō	ASP			62.449	19.947	14.789		24.38	A
ATOM	1273	N	CYS			61.352	19.277	12.935		23.95	A
ATOM	1274	CA	CYS	A	163	60.914	18.027	13.530	1.00	24.46	A
MOTA	1275	С	CYS	A	163	61.916	17.043	12.938	1.00	22.46	A
ATOM	1276	0	CYS	A	163	62.110	17.021	11.726	1.00	24.01	A
ATOM	1277	CB	CYS	Δ	163	59.497	17.658	13.083		24.14	A
	1278	SG	CYS							30.35	
MOTA						58.931	16.101	13.836			A
MOTA	1279	N	Lys			62.571	16.259	13.782	1.00	22.96	A
ATOM	1280	CA	LYS	Α	164	63.559	15.292	13.307	1.00	24.69	A
ATOM	1281	CB	LYS	A	164	64.867	15.450	14.089	1.00	27.54	A
ATOM	1282	CG	LYS			65.977	14.490	13.689		28.93	A
ATOM	1283	CD	LYS			67.179	14.643	14.622		32.03	
											A
MOTA	1284	CE	LYS			68.254	13.596	14.350		33.85	A
MOTA	1285	NZ	LYS	A	164	69.319	13.607	15.398	1.00	36.46	A
ATOM	1286	C	LYS	A	164	63.023	13.875	13.463	1.00	24.25	A
ATOM	1287	0	LYS	A	164	62.697	13.443	14.570	1.00	23.52	A
MOTA	1288	N	VAL			62.931	13.160	12.345		23.37	A
	1289	CA	VAL			62.415	11.797	12.344		24.06	A
ATOM											
ATOM	1290	CB	VAL			61.174	11.682	11.408		23.45	A
MOTA	1291	CG1	VAL	Α	165	60.657	10.248	11.382	1.00	18.80	A
ATOM	1292	CG2	VAL	Α	165	60.078	12.632	11.878	1.00	22.37	A
ATOM	1293	C	VAL	A	165	63.457	10.772	11.903	1.00	25.04	A
MOTA	1294	0			165	64.103	10.931	10.869		25.12	A
		N	GLU			63.621	9.725	12.703		26.91	A
MOTA	1295										
ATOM	1296	CA			166	64.556	8.648	12.383		28.84	A
MOTA	1297	CB	GLU	A	166	65.554	8.424	13.523	1.00	30.71	A
ATOM	1298	CG	GTA	A	166	66.382	9.634	13.922	1.00	36.90	A
ATOM	1299	CD	GLU	A	166	67.247	9.356	15.147	1.00	39.97	A
ATOM	1300		GLU			67.466	10.286	15.954	1 00	43.02	A
						67.714		15.301		43.24	A
ATOM	1301						8.206				
ATOM	1302	C	GLU			63.739	7.369	12.183		28.96	A
ATOM	1303	0	GLU	A	166	62.975	6.971	13.067	1.00	27.40	A
ATOM	1304	N	HIS	Α	167	63.910	6.728	11.029	1.00	29.87	A
ATOM	1305	CA	HIS	A	167	63.189	5.496	10.713	1.00	30.70	A
ATOM	1306	CB	HTS	Δ	167	61.838	5.833	10.084	1.00	30.90	A
ATOM	1307	CG			167	60.932	4.655	9.933		34.01	A
										33.60	
ATOM	1308		HIS			60.698	3.842	8.876			A
ATOM	1309	ND1	HIS	A	167	60.159	4.172	10.967	1.00	36.69	A
MOTA	1310	CE1	HIS	A	167	59.488	3.112	10.554	1.00	34.84	A
MOTA	1311	NE2	HIS	A	167	59.798	2.890	9.290	1.00	34.90	A
ATOM	1312	C			167	63.999	4.639	9.739		31.21	A
ATOM	1313	ŏ			167	64.696	5.167	8.866		29.44	A
MOTA	1314	N			168	63.895	3.320	9.879		31.70	A
MOTA	1315	CA			168	64.625	2.402	9.006		31.76	A
MOTA	1316	CB	TRP	A	168	64.344	0.954	9.396	1.00	30.39	A
ATOM	1317	CG	TRP	A	168	64.735	0.650	10.797	1.00	28.49	A
ATOM	1318		TRP			64.115	-0.297	11.666		28.31	A
MOTA	1319		TRP			64.837	-0.288	12.878		28.31	A
ATOM	1320		TRP			63.017	-1.157	11.538		26.47	A
ATOM	1321		TRP			65.778	1.184	11.491		28.32	A
MOTA	1322		TRP			65.849	0.627	12.744		28.98	A
ATOM	1323	CZ2	TRP	A	168	64.498	-1.107	13.958	1.00	28.85	A
ATOM	1324		TRP			62.678	-1.970	12.608	1.00	27.57	A
ATOM	1325		TRP			63.418	-1.940	13.805		29.20	A
ATOM	1326	C			168			7.523		33.06	A
						64.332	2.588				
ATOM	1327	0	IKP	A	168	65.190	2.314	6.682	1.00	32.28	A

ATOM	1328	N	GLY A	169	63.126	3.049	7.202	1.00 34.81	A
MOTA	1329	CA	GLY A		62.760	3.263	5.810	1.00 35.23	A
MOTA	1330	C	GLY A		63.267	4.588	5,266	1.00 37.25	A
ATOM	1331	0	GLY A		62.907	4.992	4.162	1.00 37.65	A
MOTA	1332	N	LEU A		64.100 64.673	5.268 6.555	6.049 5.660	1.00 39.27 1.00 41.10	A A
ATOM ATOM	1333 1334	CA CB	LEU A		64.354	7.626	6.706	1.00 38.47	A
ATOM	1335	CG	LEU A		62.923	8.143	6.843	1.00 38.66	A
ATOM	1336		LEU A		62.790	8.919	8.142	1.00 37.48	A
ATOM	1337		LEU A		62.572	9.017	5.653	1.00 37.65	A
ATOM	1338	С	LEU A	170	66.183	6.425	5.556	1.00 43.62	A
MOTA	1339	0	LEU A	170	66.809	5.762	6.382	1.00 44.45	A
MOTA	1340	N	ASP A		66.764	7.066	4.545	1.00 46.98	A
MOTA	1341	CA	ASP A		68.211	7.036	4.350	1.00 48.99	A
MOTA	1342	CB	ASP A		68.602	7.810	3.086	1.00 51.12	A A
ATOM	1343	CG	ASP A		67.735 66.520	7.466 7.761	1.895 1.936	1.00 53.30 1.00 54.82	A
MOTA MOTA	1344 1345	OD2			68.271	6.903	0.917	1.00 54.86	A
MOTA	1346	C	ASP A		68.836	7.726	5.554	1.00 48.82	A
ATOM	1347	ŏ	ASP A		69.437	7.093	6.420	1.00 48.88	A
ATOM	1348	N	LYS A		68.673	9.044	5.585	1.00 48.96	A
ATOM	1349	CA	LYS A	172	69.192	9.877	6.659	1.00 48.79	A
ATOM	1350	CB	LYS A	172	69.986	11.059	6.084	1.00 51.32	A
ATOM	1351	CG	LYS A		71.074	10.698	5.075	1.00 55.53	A
MOTA	1352	œ	LYS A		71.799	11.952	4.571	1.00 57.81	A
MOTA	1353	CE	LYS A		72.859	11.621	3.518 4.038	1.00 59.22 1.00 58.32	A A
MOTA	1354	NZ C	LYS A		73.912 67.990	10.702 10.419	7.420	1.00 46.36	Ā
ATOM ATOM	1355 1356	0	LYS A		66.862	10.381	6.919	1.00 44.39	A
ATOM	1357	N	PRO A		68.211	10.920	8.645	1.00 44.20	A
ATOM	1358	CD	PRO A		69.432	10.866	9.469	1.00 44.15	A
ATOM	1359	CA	PRO A	173	67.089	11.462	9.410	1.00 42.74	A
MOTA	1360	CB	PRO A	173	67.768	12.050	10.637	1.00 42.02	A
MOTA	1361	CG	PRO A		68.887	11.080	10.872	1.00 44.25	A
MOTA	1362	C	PRO A		66.369	12.517	8.578	1.00 41.09 1.00 39.67	A A
ATOM	1363	0	PRO A		67.002	13.309 12.502	7.877 8.636	1.00 39.80	A
ATOM	1364 1365	N CA	LEU A		65.044 64.241	13.457	7.888	1.00 38.58	A
ATOM ATOM	1366	CB	LEU A		62.894	12.838	7.522	1.00 38.73	A
ATOM	1367	CG	LEU A		62.202	13.329	6.251	1.00 39.18	A
ATOM	1368		LEU A		60.826	12.691	6.170	1.00 39.20	A
MOTA	1369	CD2	LEU A	174	62.093	14.836	6.245	1.00 40.87	A
MOTA	1370	C	LEU A		64.019	14.662	8.785	1.00 37.43	A
MOTA	1371	0	LEU A		63.630	14.514	9.943	1.00 37.68	A A
ATOM	1372	N	LEU A		64.284	15.849 17.077	8.255 9.012	1.00 35.85 1.00 34.38	A
ATOM ATOM	1373	CA CB	LEU A		64.098 65.400	17.882	9.074	1.00 33.21	A
ATOM	1374 1375	CG	LEU A		66.425	17.502	10.147	1.00 34.82	A
MOTA	1376	CD1			65.838	17.768	11.526	1.00 34.32	A
ATOM	1377		LEU A		66.819	16.038	10.008	1.00 35.37	A
ATOM	1378	C	LEU A	175	63.020	17.898	8.337	1.00 33.09	A
ATOM	1379	0	LEU A	175	63.080	18.137	7.132	1.00 33.84	A
ATOM	1380	N	LYS A		62.023	18.312	9.108	1.00 30.14	A
MOTA	1381	CA	LYS A		60.943	19.119	8.566	1.00 30.03	A
MOTA	1382	CB	LYS A		59.598	18.416 19.049	8.772 8.010	1.00 30.60 1.00 33.60	A A
MOTA	1383 1384	CD	LYS A		58.463 58.742	19.054	6.508	1.00 37.73	A
ATOM ATOM	1385	CE	LYS A		58.869	17.642	5.960	1.00 37.37	A
ATOM	1386	NZ	LYS A		59.075	17.629	4.484	1.00 41.15	A
ATOM	1387	C	LYS A		60.976	20.457	9.292	1.00 28.62	A
MOTA	1388	0	LYS A	176	60.764	20.524	10.501	1.00 27.68	A
ATOM	1389	N	HIS A		61.238	21.520	8.539	1.00 28.72	A
MOTA	1390	CA	HIS A		61.353	22.868	9.088	1.00 29.54	A
MOTA	1391	CB	HIS A		62.284	23.691	8.195	1.00 29.51 1.00 30.53	A A
ATOM	1392	CG	HIS A HIS A		62.485. 62.124	25.097 26.282	8.663 8.114	1.00 30.53	A
MOTA MOTA	1393 1394		L HIS A		63.117	25.401	9.849	1.00 32.09	A
ATOM	1395		L HIS A		63.138	26.713	10.010	1.00 32.65	A
MOTA	1396		HIS A		62.542	27.271	8.971	1.00 32.04	A
MOTA	1397	C	HIS A		60.059	23.654	9.304	1.00 29.24	A
MOTA	1398	0	HIS A		59.100	23.519	8.549	1.00 27.66	A
MOTA	1399	N	TRP A		60.062	24.492	10.340	1.00 30.09	A
ATOM	1400	CA	TRP #		58.926	25.350	10.674	1.00 33.43 1.00 28.07	A A
MOTA	1401	CB	TRP 1	A 178	57.959	24.647	11.632	a.vu 20.v/	•

ATOM	1402	CG	TRP A	A.	178	56.681	25.422	11.851	1.00 25.25	
ATOM	1403	CD2	TRP 2	A	178	56.476	26.518	12.761	1.00 21.68	3 A
MOTA	1404	CE2	TRP 2	A	178	55.138	26.942	12.611	1.00 20.86	
MOTA	1405	CE3	TRP 2	A	178	57.292	27.178	13.688	1.00 20.72	
ATOM	1406	CD1	TRP 2	A.	178	55.489	25.239	11.206	1.00 24.83	L A
ATOM	1407	NE1	TRP 2	A.	178	54.559	26.146	11.657	1.00 21.5	L A
MOTA	1408	CZ2	TRP I	A	178	54.598	27.999	13.354	1.00 21.1	l A
ATOM	1409	CZ3	TRP 2	A	178	56.754	28.229	14.428	1.00 21.5	A E
ATOM	1410	CH2	TRP 2	A	178	55.419	28.627	14.255	1.00 20.94	1 A
ATOM	1411	С	TRP 3	A	178	59.425	26.628	11.348	1.00 36.30	) A
ATOM	1412	0	TRP	A	178	60.314	26.591	12.195	1.00 36.93	1 A
ATOM	1413	N	GLU :	A	179	58.852	27.761	10.975	1.00 40.6	5 A
ATOM	1414	CA	GLU :	A	179	59.240	29.029	11.587	1.00 45.63	2 A
ATOM	1415	CB	GLU :	A	179	60.481	29.622	10.899	1.00 -47.4	2 A
ATOM	1416	CG	GLU :			60.323	29.868	9.404	1.00 52.7	7 A
ATOM	1417	CD	GLU .			61.498	30.624	8.806	1.00 55.1	7 A
MOTA	1418	OE1				62.653	30.179	8.987	1.00 57.2	0 A
ATOM	1419	OE2	GLU .			61.265	31.663	8.149	1.00 57.2	1 A
ATOM	1420	C	GLU			58.074	30.001	11.489	1.00 46.4	7 A
ATOM	1421	ō	GLU			57.322	29.983	10.513	1.00 45.4	9 A
ATOM	1422	N	PRO			57.898	30.855	12.509	1.00 47.9	7 A
ATOM	1423	CD	PRO			58.679	31.008	13.752	1.00 48.3	5 A
ATOM	1424	CA	PRO			56.789	31.810	12.460	1.00 49.4	5 A
MOTA	1425	CB	PRO			56.763	32.372	13.880	1.00 49.3	9 A
ATOM	1426	CG	PRO			58.214	32.358	14.266	1.00 48.6	
ATOM	1427	C	PRO			57.014	32.891	11.401	1.00 50.2	
	1428	Ö	PRO			58.174	33.041	10.950	1.00 49.9	
ATOM	1429	OXT				56.030	33.578	11.043	1.00 50.9	
MOTA		CB	SER		3	67.953	-2.426	7.203	1.00 59.7	
ATOM	1430 1431	OG	SER		3	68.517	-3.384	6.321	1.00 60.7	
ATOM		C	SER		3	68.164	-3.822	9.277	1.00 57.4	
ATOM	1432	0	SER		3	68.117	-4.879	8.642	1.00 57.3	
ATOM	1433	N	SER		3	70.072	-2.418	8.486	1.00 59.3	
ATOM	1434				3	68.586	-2.517	8.597	1.00 58.8	
ATOM	1435	CA	SER		4	67.855	-3.763	10.585	1.00 55.7	
MOTA	1436	И	PRO		4	67.833	-2.580	11.463	1.00 54.9	
ATOM	1437	CD	PRO		4	67.438	-4.952	11.338	1.00 53.7	
MOTA	1438	CA	PRO PRO		4	67.457	-4.467	12.787	1.00 54.7	
MOTA	1439	CB			4	67.095	-3.021	12.660	1.00 54.9	
ATOM	1440	CG	PRO			66.069	-5.487	10.918	1.00 51.0	
ATOM	1441	C	PRO		4 4	65.240	-4.753	10.379	1.00 50.9	
MOTA	1442	0	PRO		5	65.843	-6.773	11.165	1.00 47.9	
ATOM	1443	N	GLU			64.581	-7.410	10.810	1.00 45.2	
MOTA	1444	CA	GLU		5 5	64.811	-8.893	10.489	1.00 48.2	
MOTA	1445	CB	GLU		5	65.603	-9.656	11.545	1.00 54.5	_
ATOM	1446	CG	GLU		5		-11.102	11.140	1.00 57.8	_
ATOM	1447	CD	GLU.		5		-11.317	10.024	1.00 59.6	
MOTA	1448				5		-12.020	11.941	1.00 59.3	
MOTA	1449	OE2				63.548	-7.269	11.920	1.00 40.8	
ATOM	1450	C	GLU		5	63.876	-7.328	13.105	1.00 40.8	
ATOM	1451	0	GLU		5 6	62.294	-7.083	11.532	1.00 36.0	
ATOM	1452	N	ASP			61.223	-6.936	12.508	1.00 32.1	
ATOM	1453	CA	ASP			60.833	-5.460	12.616	1.00 29.9	
MOTA	1454	CB	ASP			59.933	-5.171	13.798	1.00 27.9	
MOTA	1455	CG	ASP			59.280	-4.110	13.785	1.00 29.6	
MOTA	1456		ASP			59.884	-5.982	14.745	1.00 29.8	
MOTA	1457		ASP			60.014	-7.766	12.077	1.00 29.6	
ATOM	1458	C	ASP				-7.802	10.899	1.00 29.1	
MOTA	1459	0	ASP			59.676	-8.438	13.032	1.00 27.7	
ATOM	1460	N	PHE			59.380	-9.249	12.765	1.00 28.3	
ATOM	1461	CA	PHE			58.193		13.161	1.00 29.5	
ATOM	1462	CB	PHE				-10.704	12.282	1.00 23.0	
MOTA	1463	CG	PHE				-11.385		1.00 29.8	
MOTA	1464		L PHE				-11.766	10.989	1.00 23.0	
ATOM	1465		2 PHE				-11.603	12.730 10.145	1.00 32.2	
ATOM	1466		L PHE				-12.355 -12.190	11.897	1.00 33.	
MOTA	1467						-12.190	10.599	1.00 34.	
MOTA	1468	cz	PHE					13.562	1.00 35.	
ATOM	1469		PHE			57.032 57.046	-8.657 -8.645		1.00 25.	
MOTA	1470	0	PHE				-8.174		1.00 25.	
MOTA	1471		VAL			56.023 54.891			1.00 23.	
MOTA	1472						-6.132		1.00 21.	
MOTA	1473		VAL			54.670	-5.394		1.00 21.	
MOTA	1474		1 VAL			53.573 E5 075			1.00 21.	
MOTA	1475	CG	2 VAL		8 8	55.975	9,342	ac.033		

2001	1476		VAL	-	8	53.556	-8.255	13.467	1.00 24.08	-
MOTA	1476	C								В
ATOM	1477	0	VAL		8	53.204	-8.912	12.491	1.00 23.46	В
ATOM	1478	N	TYR		9	52.804	-8.127	14.554	1.00 23.26	В
ATOM	1479	CA	TYR	В	9	51.493	-8.747	14.619	1.00 23.18	В
ATOM	1480	CB	TYR	В	9	51.510	-9.978	15.520	1.00 23.12	В
ATOM	1481	CG	TYR	В	9	50.231	-10.786	15.465	1.00 24.54	В
ATOM	1482	CD1	TYR	В	9	50.158	-11.962	14.722	1.00 26.50	В
MOTA	1483		TYR		9		-12.743	14.716	1.00 25.08	В
										В
MOTA	1484		TYR		9		-10.399	16.190	1.00 22.88	
MOTA	1485	CE2	TYR		9		-11.165	16.188	1.00 23.91	В
ATOM	1486	CZ	TYR	В	9	47.902	-12.342	15.455	1.00 24.87	В
ATOM	1487	OH	TYR	В	9	46.780	-13.140	15.501	1.00 25.45	В
ATOM	1488	C	TYR	В	9	50.509	-7.723	15.163	1.00 21.33	В
ATOM	1489	Ō	TYR		9	50.798	-7.028	16.133	1.00 22.92	В
ATOM	1490	N	GLN		10	49.353	-7.622	14.521	1.00 19.98	В
MOTA	1491	CA	GLN		10	48.326	-6.687	14.952	1.00 19.52	В
MOTA	1492	CB	GLN		10	48.171	-5.523	13.962	1.00 19.13	В
MOTA	1493	CG	GLN	В	10	49.433	-4.810	13.509	1.00 19.33	В
MOTA	1494	CD	GLN	В	10	49.117	-3.708	12.499	1.00 17.96	В
ATOM	1495	OB1	GLN	В	10	48.336	-2.802	12.783	1.00 18.49	В
MOTA	1496	NE2	GLN	В	10	49.715	-3.790	.11.316	1.00 19.41	В
ATOM	1497	C	GLN		10	46.967	-7.375	15.029	1.00 19.74	В
							-8.227	14.192	1.00 18.98	В
MOTA	1498	0	GLN		10	46.626				
ATOM	1499	N	PHE		11	46.195	-6.996	16.040	1.00 19.06	В
MOTA	1500	CA	PHE	В	11	44.842	-7.487	16.182	1.00 16.54	В
MOTA	1501	CB	PHE	В	11	44.668	-8.454	17.336	1.00 17.48	В
ATOM	1502	CG	PHE	В	11	43.237	-8.847	17.544	1.00 16.17	В
ATOM	1503	CD1	PHE	В	11	42.570	-9.604	16.582	1,00 17.49	В
ATOM	1504		PHE		11	42.536	-8.406	18.656	1.00 14.41	В
	1505		PHE		11	41.219	-9.913	16.725	1.00 18.03	В
MOTA										
MOTA	1506		PHE		11	41.191	-8.708	18.814	1.00 16.34	В
MOTA	1507	CZ	PHE		11	40.528	-9.463	17.845	1.00 17.60	В
ATOM	1508	C	PHE	В	11	43.984	-6.271	16.450	1.00 18.14	В
MOTA	1509	0	PHE	В	11	44.241	-5.506	17.386	1.00 15.63	В
ATOM	1510	N	LYS	В	12	42.961	-6.094	15.625	1.00 17.33	В
ATOM	1511	CA	LYS		12	42.082	-4.958	15.770	1.00 17.63	В
		СВ	LYS		12	42.188	-4.067	14.536	1.00 18.71	В
ATOM	1512									В
ATOM	1513	CG	LYS		12	43.599	-3.642	14.192	1.00 15.90	
MOTA	1514	Э	LYS		12	43.602	-2.909	12.871	1.00 17.33	В
ATOM	1515	CE	LYS	В	12	44.946	-2.297	12.570	1.00 18.72	В
MOTA	1516	NZ	LYS	В	12	44.838	-1.450	11.340	1.00 20.93	В
ATOM	1517	C	LYS	В	12	40.632	-5.387	15.968	1.00 18.92	В
ATOM	1518	0	LYS		12	40.041	-6.050	15.109	1.00 17.25	В
ATOM	1519	N	GLY		13	40.076	-5.002	17.114	1.00 17.59	В
										В
MOTA	1520	CA	GLY		13	38.701	-5.322	17.430	1.00 19.88	
MOTA	1521	C	GLY		13	37.874	-4.113	17.064	1.00 20.12	В
ATOM	1522	0	GLY	В	13	37.515	-3.309	17.923	1.00 21.08	В
MOTA	1523	N	MET	В	14	37.561	-4.000	15.779	1.00 20.42	В
ATOM	1524	CA	MET	В	14	36.817	-2.866	15.262	1.00 22.96	В
ATOM	1525	CB	MET	В	14	37.334	-2.554	13.866	1.00 23.02	В
ATOM	1526	CG	MET		14	38.846	-2.485	13.820	1.00 23.58	В
ATOM	1527	SD	MET		14	39.449	-2.095	12.191	1.00 26.23	В
								12.182		
ATOM	1528	CE	MET		14	39.260	-0.318		1.00 25.78	В
ATOM	1529	C	MET		14	35.295	-2.997	15.242	1.00 23.12	В
ATOM	1530	0	MET	В	14	34.751	-4.089	15.081	1.00 24.36	В
ATOM	1531	N	CYS	В	15	34.628	-1.860	15.427	1.00 24.04	В
MOTA	1532	CA	CYS	В	15	33.173	-1.768	15.433	1.00 24.91	В
MOTA	1533	C	CYS		15	32.808	-0.587	14.547	1.00 25.49	В
ATOM	1534	ō	CYS		15	33.369	0.504	14.700	1.00 23.97	В
						32.630		16.847	1.00 26.02	В
ATOM	1535	CB	CYS		15					
ATOM	1536	SG	CYS		15	32.691		18.084	1.00 33.69	В
MOTA	1537	N	TYR	. В	16	31.871		13.630	1.00 25.87	В
ATOM	1538	CA	TYR	В	16	31.413	0.244	12.724	1.00 25.59	В
ATOM	1539	CB	TYR	В	16	31.539	-0.223	11.274	1.00 24.73	В
MOTA	1540	CG	TYR	В	16	32.958	-0.575	10.879	1.00 26.05	В
MOTA	1541		TYR		16	33.523		11.239	1.00 22.96	В
ATOM	1542				16	34.843		10.904	1.00 25.81	В
			TYR							В
ATOM	1543		TYR		16	33.748		10.171	1.00 25.30	
MOTA	1544	CE2			16	35.066		9.835	1.00 25.12	В
MOTA	1545	$\mathbf{cz}$	TYR		16	35.607		10.202	1.00 26.66	B
ATOM	1546	OH	TYR	В	16	36.908		9.868	1.00 29.22	В
ATOM	1547	С	TYR	В	16	29.960	0.575	13.045	1.00 26.48	В
ATOM	1548	ō	TYP		16	29.113		13.091	1.00 26.41	В
ATOM	1549	N	PHE		17	29.684		13.266	1.00 27.76	В
			- 110	د .			2.000			_

ATOM	1550	CA	PHE B	17	28.346	2.338	13.613	1.00 29.09	В
ATOM	1551	CB	PHE B	17	28.382	3.047	14.967	1.00 28.08	В
ATOM	1552	CG	PHE B	17	28.885	2.194	16.091	1.00 28.21	В
ATOM	1553		PHE B		28.056	1.253	16.693	1.00 27.20	В
MOTA	1554		PHE B		30.188	2.340	16.558	1.00 26.60	В
ATOM	1555		PHE B		28.519	0.470	17.752	1.00 28.13	В
			PHE B		30.662	1.565	17.610	1.00 25.62	В
MOTA	1556						18.210	1.00 25.02	В
MOTA	1557	,cz	PHE B		29.828	0.629			В
MOTA	1558	C	PHE B		27.772	3.318	12.592	1.00 30.71	
ATOM	1559	0	PHE B		28.452	4.239	12.155	1.00 31.05	В
ATOM	1560	N	THR B	18	26.506	3.125	12.237	1.00 33.51	В
MOTA	1561	CA	THR B	18	25.831	4.005	11.291	1.00 36.95	В
MOTA	1562	CB	THR B	18	25.797	3.395	9.875	1.00 37.23	В
MOTA	1563	OG1	THR B	18	27.133	3.105	9.447	1.00 40.77	В
ATOM	1564	CG2	THR B	18	25.171	4.369	8.891	1.00 38.43	В
ATOM	1565	C	THR E		24.398	4.273	11.753	1.00 38.56	В
ATOM	1566	ō	THR E		23.671	3.351	12.131	1.00 38.36	В
ATOM	1567	N	ASN E		24.007	5.544	11.726	1.00 39.80	В
			ASN E		22.668	5.961	12.132	1.00 41.35	В
ATOM	1568	CA				5.465	11.110	1.00 41.21	В
MOTA	1569	CB	ASN E		21.638			1.00 42.85	В
ATOM	1570	CG	ASN E		20.311	6.190	11.223		
ATOM	1571		ASN E		20.271	7.378	11.548	1.00 42.24	В
ATOM	1572	ND2	ASN E		19.219	5.485	10.937	1.00 42.57	В
ATOM	1573	C	ASN E	3 19	22.352	5.416	13.521	1.00 42.37	В
ATOM	1574	0	ASN E	3 19	21.540	4.503	13.673	1.00 43.36	В
ATOM	1575	N	GLY E	3 20	22.997	5.989	14.533	1.00 42.56	В
ATOM	1576	CA	GLY E	3 20	22.790	5.535	15.894	1.00 43.89	В
ATOM	1577	С	GLY E	3 20	23.293	4.110	16.031	1.00 45.10	В
MOTA	1578	0	GLY F	3 20	24.421	3.807	15.646	1.00 44.28	В
MOTA	1579	N	THR I		22.458	3.232	16.575	1.00 46.37	В
ATOM	1580	CA	THR I		22.824	1.832	16.738	1.00 47.42	В
ATOM	1581	СВ	THR I		22.667	1.373	18.199	1.00 48.57	В
			THR I		21.438	1.885	18.731	1.00 49.14	В
ATOM	1582				23.843	1.856	19.043	1.00 47.59	В
ATOM	1583		THR I				15.846	1.00 48.74	В
MOTA	1584	C	THR 1		21.958	0.947		1.00 48.04	В
MOTA	1585	0	THR I		21.925	-0.276	16.016		
MOTA	1586	N	GLU 1		21.253	1.570	14.902	1.00 48.57	В
MOTA	1587	CA	GLU 1		20.405	0.822	13.979	1.00 48.90	В
ATOM	1588	CB	GLU 1	B 22	19.741	1.745	12.957	1.00 52.60	В
ATOM	1589	CG	GLU 1	B 22	18.669	2.667	13.493	1.00 58.06	В
MOTA	1590	æ	GLU I	B 22	17.862	3.297	12.368	1.00 62.27	В
ATOM	1591	OE1	GLU :	B 22	17.027	4.185	12.648	1.00 63.99	В
ATOM	1592	OE2	GLU I	B 22	18.065	2.894	11.199	1.00 64.70	В
ATOM	1593	C	GLU :		21.285	-0.156	13.229	1.00 46.38	В
ATOM	1594	0	GLU :	B 22	21.029	-1.356	13.209	1.00 45.52	В
ATOM	1595	N	ARG :		22.324	0.379	12.601	1.00 45.42	В
ATOM	1596	CA	ARG		23.260	-0.438	11.844	1.00 44.59	В
MOTA	1597	CB	ARG		23.423	0.127	10.422	1.00 45.69	В
ATOM	1598		ARG		22.169	-0.062	9.554	1.00 49.95	В
		CG			22.406	0.237	8.074	1.00 53.34	В
MOTA	1599	CD	ARG		22.153	1.632	7.708	1.00 55.57	В
ATOM	1600	NE	ARG				7.700	1.00 57.20	В
ATOM	1601	CZ	ARG		20.949	2.200	8.042	1.00 58.09	В
MOTA	1602		ARG		19.878	1.495	7.340	1.00 56.82	В
MOTA	1603		ARG		20.813	3.471			
MOTA	1604	С	ARG		24.606	-0.534	12.567	1.00 40.56	В
MOTA	1605	0	ARG	B 23	25.306	0.459	12.748	1.00 41.15	В
MOTA	1606	N	VAL	B 24	24.944	-1.743	12.995	1.00 38.17	В
MOTA	1607	CA	VAL	B 24	26.191	-1.996	13.708	1.00 34.88	В
MOTA	1608	CB	VAL	B 24	25.931	-2.314	15.200	1.00 34.41	В
MOTA	1609	CG1	VAL	B 24	27.251	-2.526	15.918	1.00 35.28	В
MOTA	1610	CG2	. VAL	B 24	25.146	-1.190	15.852	1.00 34.70	В
ATOM	1611	C	VAL	B 24	26.909	-3.194	13.100	1.00 32.34	В
ATOM	1612	o	VAL		26.287	-4.214	12.812	1.00 33.23	В
ATOM	1613	N	ARG		28.217	-3.076	12.898	1.00 30.18	В
ATOM	1614	CA	ARG		28.970	-4.194	12.354	1.00 26.97	В
ATOM	1615	CB	ARG		29.225	-4.022	10.852	1.00 27.67	В
			ARG		29.400	-5.362	10.170	1.00 29.58	В
ATOM	1616	CG			30.406	-5.363	9.052	1.00 31.26	В
MOTA	1617	CD	ARG			-4.454	7.974	1.00 33.12	В
MOTA	1618	NE	ARG				6.705	1.00 33.12	В
ATOM	1619	CZ	ARG			-4.631	6.346	1.00 32.27	В
MOTA	1620		l ARG			-5.695		1.00 31.13	В
ATOM	1621		2 ARG			-3.726	5.799		В
MOTA	1622		ARG			-4.402	13.065	1.00 24.10	В
ATOM	1623	0	ARG	B 25	31.095	-3.477	13.225	1.00 22.56	٥

ATOM	1624	N	LEU	В	26	30.551	-5.630	13.495	1.00 22.65	В
MOTA	1625	CA	LEU	В	26	31.801	-5.942	14.163	1.00 22.38	В
ATOM	1626	CB	LEU		26	31.558	-6.888	15.345	1.00 20.25	В
MOTA	1627	CG	LEU		26	32.795	-7.389	16.100	1.00 19.86	В
MOTA	1628		LEU		26	32.452	-7.613	17.568	1.00 22.49	В
ATOM	1629	CD2	LEU	В	26	33.304	-8.665	15.464	1.00 18.43	В
MOTA	1630	С	LEU	В	26	32.726	-6.591	13.150	1.00 21.50	В
ATOM	1631	0	LEU	В	26	32.289	-7.402	12.342	1.00 22.83	В
ATOM	1632	N	VAL		27	33.998	-6.208	13.177	1.00 21.29	В
ATOM	1633	CA	VAL		27	34.984	-6.780	12.270	1.00 20.66	В
MOTA	1634	CB	VAL	В	27	35.178	-5.911	11.004	1.00 20.59	В
MOTA	1635	CG1	VAL	В	27	36.169	-6.576	10.069	1.00 19.45	В
ATOM	1636	CG2	VAL	В	27	33.849	-5.696	10.297	1.00 22.37	В
ATOM	1637	C	VAL		27	36.330	-6.885	12.988	1.00 22.39	В
										В
ATOM	1638	0	VAL		27	37.046	-5.889	13.135	1.00 22.63	
MOTA	1639	N	SER	В	28	36.673	-8.083	13.450	1.00 21.32	В
ATOM	1640	CA	SER	В	28	37.947	-8.259	14.130	1.00 21.51	В
ATOM	1641	CB	SER	В	28	37.831	-9.284	15.275	1.00 19.72	В
ATOM	1642	OG	SER		28		-10.581	14.819	1.00 24.33	В
									1.00 21.25	В
MOTA	1643	C	SER		28	38.954	-8.693	13.074		
ATOM	1644	0	SER	В	28	38.661	-9.537	12.229	1.00 19.44	В
ATOM	1645	N	ARG	В	29	40.137	-8.089	13.106	1.00 20.61	В
ATOM	1646	CA	ARG	В	29	41.158	-8.402	12.115	1.00 19.66	В
ATOM	1647	CB	ARG	В	29	41.418	-7.169	11.230	1.00 19.91	В
	1648	CG	ARG		29	40.178	-6.407	10.754	1.00 16.79	В
ATOM										
ATOM	1649	CD	ARG		29	40.608	-5.121	10.031	1.00 18.10	В
ATOM	1650	NE	ARG	В	29	39.487	-4.318	9.553	1.00 19.38	В
ATOM	1651	CZ	ARG	В	29	38.738	-4.619	8.497	1.00 20.62	В
ATOM	1652	NH1	ARG	В	29	38.983	-5.714	7.789	1.00 19.50	В
	1653	NH2	ARG		29	37.736	-3.822	8.149	1.00 21.90	В
ATOM									1.00 18.57	В
MOTA	1654	C	ARG		29	42.482	-8.833	12.738		
ATOM	1655	0	ARG	В	29	43.024	-8.121	13.584	1.00 19.40	В
ATOM	1656	N	SER	В	30	42.991	-9.995	12.326	1.00 18.99	В
ATOM	1657	CA	SER	В	30	44.284	-10.501	12.797	1.00 21.66	В
ATOM	1658	СВ	SER		30		-12.015	13.023	1.00 22.77	В
					30		-12.352	14.106	1.00 26.81	В
MOTA	1659	OG	SER							
ATOM	1660	C	SER		30		-10.163	11.673	1.00 23.37	В
MOTA	1661	0	SER	В	30	45.055	-10.553	10.522	1.00 21.31	В
MOTA	1662	N	ILE	В	31	46.338	-9.450	12.009	1.00 24.76	В
ATOM	1663	CA	ILE		31	47.298	-8.998	10.999	1.00 24.33	В
		СВ	ILE		31	47.341	-7.440	10.958	1.00 25.20	В
MOTA	1664									
MOTA	1665		ILE		31	47.982	-6.964	9.672	1.00 23.24	В
ATOM	1666	CG1	ILE	В	31	45.934	-6.857	11.106	1.00 26.96	В
MOTA	1667	CD1	ILE	В	31	45.032	-7.136	9.947	1.00 31.25	В
ATOM	1668	С	ILE	В	31	48.741	-9.460	11.187	1.00 23.98	В
	1669	ō	ILE		31	49.298	-9.318	12.272	1.00 22.29	В
MOTA									1.00 25.50	В
MOTA	1670	N	TYR		32	49.345	-9.993	10.123		
MOTA	1671	CA	TYR	. В	32		-10.405	10.162	1.00 26.21	В
MOTA	1672	CB	TYR	В	32	50.965	-11.764	9.492	1.00 28.46	В
ATOM	1673	CG	TYR	В	32	52.406	-12.224	9.544	1.00 31.10	В
MOTA	1674		TYR		32		-12.412	10.765	1.00 32.47	В
					32			10.827	1.00 34.69	В
MOTA	1675		TYR				-12.780			
MOTA	1676		TYR		32		-12.424	8.375	1.00 33.60	В
MOTA	1677	CE2	TYR	В	32	54.484	-12.795	8.422	1.00 34.50	В
MOTA	1678	$\mathbf{cz}$	TYR	В	32	55.103	-12.965	9.654	1.00 35.65	В
MOTA	1679	OH	TYR		32	56.438	-13.281	9.717	1.00 37.73	В
ATOM	1680	C	TYR		32	51.478	-9.307	9.384	1.00 25.67	В
							-9.140	8.174	1.00 24.75	В
MOTA	1681	0	TYR		32	51.273				
ATOM	1682	N	asn	В	33	52.319	-8.559	10.094	1.00 25.63	В
MOTA	1683	CA	asn	В	33	53.036	-7.416	9.526	1.00 24.95	В
MOTA	1684	CB	ASN	ГВ	33	53.955	-7.848	8.379	1.00 23.75	В
MOTA	1685	CG	ASN		33	55.171	-8.615	8.878	1.00 24.11	В
ATOM			ASN		33	55.803	-8.223	9.861	1.00 25.42	В
	1686								1.00 25.12	В
ATOM	1687		2 ASN		33	55.506		8.204		
MOTA	1688	C	asn		33	51.990		9.070	1.00 25.11	В
MOTA	1689	0	ASN	ΙB	33	51.491	-5.618	9.893	1.00 26.06	В
ATOM	1690	'N	ARG			51.652		7.786	1.00 25.75	В
MOTA	1691	CA	ARG		34	50.631		7.296	1.00 27.64	В
					34	51.244		6.408	1.00 27.74	В
MOTA	1692	CB	ARG						1.00 29.94	В
MOTA	1693	CG	ARG		34	51.972		7.158		
MOTA	1694	CD	ARG	3 B	34	51.664		6.541	1.00 32.95	В
MOTA	1695	NE	ARG	В	34	51.897	-1.875	5.101	1.00 35.17	В
MOTA	1696	CZ	ARG		34	51.392	-0.973	4.267	1.00 37.51	В
MOTA	1697		L ARC		34	50.622		4.729	1.00 39.45	В
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ATOM	1698	NH2	ARG	В	34	51.642	-1.058	2.967	1.00 36.90	В
ATOM	1699	C	ARG		34	49.587	-6.218	6.498	1.00 26.48	В
ATOM	1700	ō	ARG		34	48.740	-5.639	5.825	1.00 27.17	В
ATOM	1701	N	GLU		35	49.647	-7.534	6.602	1.00 25.66	В
ATOM	1702	CA	GLU		35		-8.394	5.867	1.00 26.99	В
ATOM	1703	CB	GLU		35	49.570	-9.483	5.175	1.00 31.53	В
MOTA	1704	CG	GLU		35	48.814	-10.396	4.235	1.00 36.29	В
MOTA	1705	CD	GLU		35		-11.530	3.731	1.00 40.61	В
MOTA	1706		GLU		35	50.825	-11.240	3.276	1.00 45.20	В
MOTA	1707		GLU		35	49.266	-12.705	3.791	1.00 41.13	В
ATOM	1708	С	GĽΩ	В	35	47.699	-9.031	6.764	1.00 25.09	В
ATOM	1709	0	GLU	В	35	48.028	-9.807	7.663	1.00 23.31	В
ATOM	1710	N	GLU	В	36	46.439	-8.689	6.522	1.00 24.53	В
ATOM	1711	CA	GLU	В	36	45.332	-9.263	7.275	1.00 25.73	В
MOTA	1712	CB	GLU	В	36	44.023	-8.519	6.958	1.00 26.62	В
MOTA	1713	CG	GLU	В	36	42.783	-9.095	7.636	1.00 28.26	В
ATOM	1714	CD	GΓΩ	В	36	41.545	-8.232	7.442	1.00 31.08	В
ATOM	1715	OE1	GLU	В	36	41.420	-7.590	6.377	1.00 32.56	В
ATOM	1716	OE2	GLU	В	36	40.685	-8.206	8.349	1.00 32.83	В
ATOM	1717	C	GLU		36		-10.717	6.822	1.00 24.67	В
MOTA	1718	0	GLU		36		-10.992	5.626	1.00 23.91	В
MOTA	1719	N	ILE		37		-11.647	7.771	1.00 26.11	В
ATOM	1720	CA	ILE		37		-13.067	7.433	1.00 27.80	В
ATOM	1721	CB	ILE		37		-13.822	8.013	1.00 27.27	В
ATOM	1722		ILE		37		-13.174	7.516	1.00 27.41	В
ATOM	1723		ILE		37		-13.767	9.537	1.00 29.35	В
ATOM	1724		ILE		37		-14.509	10.175	1.00 30.27	B B
ATOM	1725	C	ILE		37		-13.750	7.879	1.00 27.86 1.00 28.29	В
ATOM	1726	0	ILE		37		-14.674	7.221 8.989	1.00 28.29	В
ATOM	1727	N	VAL		38		-13.296 -13.870	9.487	1.00 29.29	В
ATOM	1728	CA	VAL VAL		38 38		-14.751	10.741	1.00 30.18	В
ATOM	1729 1730	CB	VAL		38		-15.452	11.071	1.00 33.17	В
ATOM ATOM	1731		VAL		38		-15.764	10.520	1.00 31.09	В
MOTA	1732	C	VAL		38		-12.745	9.882	1.00 28.75	В
ATOM	1733	0	VAL		38		-11.758	10.480	1.00 29.70	В
ATOM	1734	N	ARG		39		-12.911	9.581	1.00 27.05	В
ATOM	1735	CA	ARG		39		-11.890	9.892	1.00 25.46	В
ATOM	1736	CB	ARG		39		-11.064	8.632	1.00 27.23	В
MOTA	1737	CG	ARG		39		-10.011	8.765	1.00 30.84	В
MOTA	1738	CD	ARG		39	37.111			1.00 29.34	В
ATOM	1739	NE	ARG		39	38.218		6.673	1.00 30.83	В
ATOM	1740	CZ	ARG		39	38.116		5.459	1.00 31.23	В
MOTA	1741		ARG		39	36.951		4.823	1.00 31.08	В
MOTA	1742		ARG		39	39.178	-7.779	4.883	1.00 30.81	В
ATOM	1743	C	ARG	В	39	37.573	-12.476	10.381	1.00 25.41	В
ATOM	1744	0	ARG	В	39	37.192	-13.587	9.996	1.00 25.06	В
ATOM	1745	N	PHE	В	40	36.890	-11.742	11.252	1.00 23.72	В
MOTA	1746	CA	PHE	В	40	35.569	-12.164	11.696	1.00 24.04	В
ATOM	1747	CB	PHE	В	40	35.498	-12.554	13.171	1.00 22.69	В
MOTA	1748	CG	PHE		40		-13.036	13.573	1.00 20.75	В
MOTA	1749		PHE		40		-14.370	13.413	1.00 21.07	В
MOTA	1750		PHE		40		-12.135	14.003	1.00 21.00	В
MOTA	1751		PHE		40		-14.800	13.670	1.00 20.86	В
MOTA	1752		PHE		40		-12.553	14.261	1.00 19.95	В
MOTA	1753	$\mathbf{cz}$	PHE		40		-13.890	14.092	1.00 19.78	В
MOTA	1754	С	PHE		40	34.662		11.474	1.00 24.27	В
MOTA	1755	0	PHE		40	34.755		12.183	1.00 22.94 1.00 24.75	B B
MOTA	1756	N	ASP		41	33.800		10.471	1.00 24.75	В
MOTA	1757	CA	ASP		41	32.857		10.101 8.578	1.00 25.64	В
MOTA	1758	CB	ASP		41	32.863		8.116	1.00 27.70	В
MOTA	1759	CG	ASP ASP		41 41	32.162 31.163		8.749	1.00 27.70	В
MOTA	1760		. ASP		41	32.607		7.102	1.00 30.42	В
MOTA	1761		ASP ASP		41		7 -10.497	10.560	1.00 24.50	В
MOTA MOTA	1762 1763	0	ASP		41		L ~11.558	10.151	1.00 24.95	В
ATOM	1764	N	SBR		42	30.822		11.404	1.00 24.16	В
MOTA	1765	CA	SER		42		L -10.096	11.882	1.00 26.13	В
ATOM	1766	CB	SER		42	29.013		12.972	1.00 24.53	В
ATOM	1767	OG	SER		42	28.932		12.497	1.00 23.39	В
ATOM	1768	c	SEF		42		7 -10.149	10.729	1.00 27.68	В
ATOM	1769	ŏ	SEF		42		1 -10.833	10.818	1.00 27.31	В
ATOM	1770	N	ASI		43	28.789		9.654	1.00 28.17	В
ATOM	1771	CA	ASI		43	27.92		8.477	1.00 29.40	В

MOTA	1772	CB	ASP B	43	28.332	-8.298	7.508	1.00 29.57	В
ATOM	1773	CG	ASP B	43	27.587	-7.006	7.766	1.00 32.71	В
ATOM	1774		ASP B	43	26.999	-6.868	8.862	1.00 33.94	В
ATOM	1775		ASP B	43	27.593	-6.120	6.881	1.00 33.98	В
					28.036 -		7.782	1.00 29.46	В
ATOM	1776	C	ASP B	43					В
MOTA	1777	0	ASP B	43	27.162 -		7.009	1.00 30.77	
MOTA	1778	N	VAL B	44	29.123 -		8.068	1.00 27.98	В
ATOM	1779	CA	VAL B	44	29.365 -	12.780	7.486	1.00 27.16	В
MOTA	1780	CB	VAL B	44	30.846 -	12.939	7.075	1.00 27.32	В
MOTA	1781		VAL B	44	31.083 -		6.488	1.00 24.09	В
			VAL B	44	31.218 -		6.073	1.00 24.66	В
MOTA	1782								
MOTA	1783	C	VAL B	44	28.990 -		8.490	1.00 28.43	В
ATOM	1784	0	VAL B	44	28.558 -	-14.948	8.108	1.00 29.45	В
ATOM	1785	N	GLY B	45	29.177 -	-13.590	9.774	1.00 28.05	В
MOTA	1786	CA	GLY B	45	28.794 -	-14.561	10.780	1.00 28.67	В
ATOM	1787	c	GLY B	45	29.758 -		11.125	1.00 28.25	В
					29.458		12.002	1.00 29.67	В
MOTA	1788	0	GLY B	45					В
ATOM	1789	N	GLU B	46	30.895 -		10.443	1.00 27.03	
ATOM	1790	CA	GLU B	46	31.873 -	-16.787	10.757	1.00 29.26	В
ATOM	1791	CB	GLU B	46	31.571 -	-18.087	10.000	1.00 32.16	В
ATOM	1792	CG	GLU B	46	32.039	-18.121	8.554	1.00 37.36	В
	1793	CD	GLU B	46	31.752		7.885	1.00 41.59	В
ATOM					32.163		8.433	1.00 43.30	В
ATOM	1794		GLU B	46					В
MOTA	1795	OE2	GLU B	46	31.116 ·		6.810	1.00 43.54	
ATOM	1796	C	GLU B	46	33.272	-16.295	10.413	1.00 29.29	В
ATOM	1797	0	GLU B	46	33.432	-15.288	9.722	1.00 30.45	В
ATOM	1798	N	PHE B	47	34.281	-17.005	10.904	1.00 28.00	В
	1799	CA	PHE B	47	35.670		10.651	1.00 28.10	В
ATOM					36.594		11.566	1,00 28.74	В
ATOM	1800	CB	PHE B	47					В
ATOM	1801	CG	PHE B	47	36.487		13.016	1.00 30.23	
MOTA	1802	CD1	PHE B	47	37.248	-16.023	13.535	1.00 28.96	В
ATOM	1803	CD2	PHE B	47	35.636	-17.768	13.870	1.00 30.80	В
ATOM	1804		PHE B	47	37.166	-15.683	14.888	1.00 31.59	В
			PHE B	47	35.544		15.229	1.00 31.97	В
MOTA	1805						15.737	1.00 30.36	В
ATOM	1806	$\mathbf{cz}$	PHE B	47	36.311				В
ATOM	1807	C	PHE B	47	36.034		9.211	1.00 28.71	
ATOM	1808	0	PHE B	47	35.576	-17.937	8.640	1.00 28.03	В
ATOM	1809	N	ARG B	48	36.872	-16.091	8.637	1.00 27.96	В
MOTA	1810	CA	ARG B	48	37.327	-16.242	7.261	1.00 26.41	В
		СВ	ARG B	48	36.513		6.326	1.00 26.57	В
ATOM	1811				35.068		6.108	1.00 26.19	В
MOTA	1812	CG	ARG B	48				1.00 24.98	В
MOTA	1813	CD	ARG B	48	34.971		5.352		
ATOM	1814	NB	arg b	48	33.579	-17.465	5.146	1.00 26.01	В
MOTA	1815	$\mathbf{cz}$	ARG B	48	32.755	-16.867	4.294	1.00 26.84	В
MOTA	1816	NH1	ARG B	48	33.181	-15.857	3.554	1.00 26.92	В
ATOM	1817		ARG B	48	31.492	-17.260	4.204	1.00 30.22	В
		C	ARG B	48	38.799		7.140	1.00 26.95	В
MOTA	1818						7.737	1.00 24.36	В
ATOM	1819	0	ARG B	48	39.255				
ATOM	1820	N	ALA B	49		-16.647	6.373	1.00 24.93	В
ATOM	1821	CA	ALA B	49	40.943	-16.349	6.143	1.00 26.58	В
ATOM	1822	CB	ALA B	49	41.709	-17.619	5.792	1.00 27.05	В
ATOM	1823	С	ALA B	49	40.927	-15.397	4.956	1.00 26.47	В
ATOM	1824	ō	ALA B			-15.635	3.983	1.00 26.12	В
			VAL B			-14.302	5.044	1.00 27.06	В
MOTA	1825	N				-13.357	3.936	1.00 26.50	В
MOTA	1826	CA	VAL B					1.00 27.14	В
MOTA	1827	CB	VAL B			-11.876	4.439		
ATOM	1828		L VAL B			-11.827	5.846	1.00 29.89	В
MOTA	1829	CG	VAL B	50	42.628	-11.020	3.501	1.00 27.33	В
MOTA	1830	C	VAL B	50	42.891	-13.742	3.037	1.00 26.58	В
MOTA	1831	ō	VAL B		42.914	-13.390	1.860	1.00 27.84	В
		N	THR B			-14.489	3.598	1.00 26.61	В
MOTA	1832					-15.011	2.846	1.00 28.59	В
MOTA	1833	CA	THR E					1.00 28.25	В
MOTA	1834	СВ	THR B			-14.193	3.056		
MOTA	1835		1 THR E			-14.464	4.356	1.00 28.56	В
MOTA	1836	CG:	2 THR E	51	46.033	-12.699	2.899	1.00 27.40	В
MOTA	1837		THR E		45.256	-16.435	3.344	1.00 29.29	В
MOTA	1838		THR E			-16.818	4.418	1.00 30.16	В
			LEU E			-17.217	2.575	1.00 30.64	В
ATOM	1839						2.959	1.00 31.32	В
MOTA	1840					-18.596		1.00 32.19	В
MOTA	1841					-19.237	1.963		
MOTA	1842	CG	LEU E			-19.724	0.624	1.00 36.90	В
ATOM	1843	CD	1 LEU E	3 52	47.836	-20.306	-0.216	1.00 35.68	В
ATOM	1844		2 LEU I		45.620	-20,775	0.861	1.00 35.34	В
ATOM	1845		LEU I			-18.724	4.359	1.00 31.57	В
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ATOM	1846	0	LEU B	52	46.570 -19.656	5.097	1.00 31.50	В
ATOM	1847	N	LEU B	53	47.753 -17.78		1.00 31.09	В
MOTA	1848	CA	LEU B	53	48.388 -17.819		1.00 30.93	В
ATOM	1849	CB	LEU B	53	49.160 -16.51		1.00 31.99	В
ATOM	1850	CG	TER B	53 53	50.338 -16.533 51.364 -17.55		1.00 35.20 1.00 35.92	B B
ATOM	1851		LEU B	53 53	50.975 -15.14		1.00 34.96	В
ATOM ATOM	1852 1853	C	LEU B		47.377 -18.01		1.00 29.90	В
ATOM	1854	ō	LEU B		47.663 -18.70		1.00 30.68	В
ATOM	1855	N	GLY B		46.192 -17.43		1.00 28.63	В
ATOM	1856	CA	GLY B		45.181 -17.53	7 8.057	1.00 29.75	В
ATOM	1857	C	GLY B	54	44.140 -18.63	7.901	1.00 30.44	В
ATOM	1858	0	GLY B	54	43.146 -18.66		1.00 28.02	В
ATOM	1859	N	TEA B		44.364 -19.54		1.00 30.54	В
MOTA	1860	CA	TEO B		43.417 -20.63		1.00 32.59	В
ATOM	1861	CB	TEO B		43.765 -21.34		1.00 35.94	B B
ATOM	1862	CG	FEA B		42.776 -22.38 41.355 -21.83		1.00 38.88 1.00 38.23	В
MOTA MOTA	1863 1864		PEO B		43.173 -22.76		1.00 39.03	В
ATOM	1865	C	LEU B		43.330 -21.63		1.00 32.20	В
ATOM	1866	ō	LEU B		42,235 -22.02		1.00 33.32	В
MOTA	1867	N	PRO B		44.478 -22.05	8 8.447	1.00 31.03	В
MOTA	1868	CD	PRO B	56	45.862 -21.80	2 8.009	1.00 30.17	В
MOTA	1869	CA	PRO B	56	44.451 -23.01		1.00 30.23	В
MOTA	1870	CB	PRO B		45.925 -23.14		1.00 30.27	В
MOTA	1871	CG	PRO B		46.609 -22.96		1.00 28.92	В
MOTA	1872	C	PRO E		43.613 -22.52		1.00 31.42 1.00 33.17	B B
ATOM	1873	0	PRO E		42.730 -23.23 43.893 -21.30		1.00 30.04	В
ATOM	1874 1875	N CA	ALA E		43.181 -20.71		1.00 28.60	В
ATOM ATOM	1876	CB	ALA E		43.818 -19.38		1.00 26.81	В
ATOM	1877	C	ALA E		41.695 -20.52		1.00 29.08	В
ATOM	1878	ō	ALA E		40.847 -20.73		1.00 28.22	В
ATOM	1879	N	ALA E	58	41.385 -20.13	5 10.791	1.00 28.84	В
ATOM	1880	CA	ALA E	58	40.002 -19.92		1.00 31.06	В
MOTA	1881	CB	ALA E		39.955 -19.42		1.00 29.79	В
ATOM	1882	C	ALA E		39.169 -21.19		1.00 32.38	В
MOTA	1883	0	ALA E		38.113 -21.19		1.00 31.57.	B B
MOTA	1884	N	GLU E		39.647 -22.28		1.00 33.50 1.00 33.91	В
ATOM	1885	CA	GLU E		38.949 -23.56 39.706 -24.62		1.00 35.67	В
MOTA MOTA	1886 1887	CB	GLU E		39.619 -24.45		1.00 39.73	В
ATOM	1888	CD	GLU I		40.327 -25.58		1.00 43.58	В
ATOM	1889		GLU		41.561 -25.71		1.00 44.52	В
MOTA	1890	OE2	GLU I	3 59	39.648 -26.33	7 6.222	1.00 44.30	В
ATOM	1891	C	GLU I	3 59	38.771 -24.06		1.00 33.56	В
MOTA	1892	0	GLU I	3 59	37.708 -24.57		1.00 34.40	В
MOTA	1893	N	TYR I		39.815 -23.92		1.00 31.99	В
MOTA	1894	CA	TYR I		39.754 -24.36		1.00 31.01	B B
ATOM	1895	CB	TYR I		41.112 -24.20 41.051 -24.54		1.00 31.13	В
MOTA	1896	CG	TYR I L TYR I		40.919 -25.87		1.00 32.55	В
MOTA	1897 1898		LTYRI		40.770 -26.19		1.00 35.39	В
MOTA MOTA	1899		2 TYR 1		41.039 -23.55		1.00 32.67	В
ATOM	1900		2 TYR		40.890 -23.85		1.00 35.14	В
ATOM	1901	CZ	TYR		40.756 -25.17		1.00 36.91	В
ATOM	1902	OH	TYR I	B 60	40.606 -25.48	3 19.791	1.00 40.06	В
ATOM	1903	C	TYR I	B 60	38.695 -23.63		1.00 31.72	В
MOTA	1904	0	TYR :		37.840 -24.25		1.00 31.72	В
MOTA	1905	N	TRP		38.752 -22.30		1.00 30.37	В
ATOM	1906	CA	TRP		37.790 -21.52		1.00 31.57	B
MOTA	1907	CB	TRP		38.129 -20.03 39.430 -19.6		1.00 32.14	В
MOTA	1908 1909	CG.	TRP :		40.359 -18.6		1.00 35.75	В
MOTA MOTA	1910		2 TRP		41.418 -18.60		1.00 35.99	В
ATOM	1911		3 TRP		40.397 -17.7		1.00 38.30	В
ATOM	1912		1 TRP		39.949 -20.2		1.00 33.63	В
MOTA	1913		1 TRP		41.142 -19.6		1.00 33.97	В
ATOM	1914		2 TRP		42.512 -17.7			В
MOTA	1915		3 TRP		41.487 -16.8			В
ATOM	1916		2 TRP		42.527 -16.8			B B
MOTA	1917		TRP		36.349 -21.7 35.436 -21.7			B
MOTA	1918		TRP ASN		36.137 -21.9			В
MOTA	1919	N	MON	02 د	30.137 -21.3		1.00 31.03	

MOTA	1920	CA	asn b	62	34.781 -22.191 12.	950 1.00 32.57 B
ATOM	1921	CB	asn b	62	34.701 -22.021 11.	434 1.00 30.37 · B
ATOM	1922	CG	ASN B	62	34.575 -20.574 11.	025 1.00 29.69 B
ATOM	1923		ASN B	62	33.889 -19.794 11.	680 1.00 29.42 B
			ASN B	62		926 1.00 31.50 B
ATOM	1924					
MOTA	1925	C	asn b	62		339 1.00 32.87 B
ATOM	1926	0	asn b	62	33.028 -23.789 13.	292 1.00 34.70 B
ATOM	1927	N	SER B	63	35,128 -24,469 13.	725 1.00 32.43 B
ATOM	1928	CA	SER B	63		140 1.00 32.38 B
ATOM	1929	CB	SER B	63		
MOTA	1930	OG	SER B	63		760 1.00 33.33 B
MOTA	1931	С	SER B	63	34.348 -25.768 15.	630 1.00 32.14 B
ATOM	1932	0	SER B	63	33.677 -26.667 16.	138 1.00 32.86 B
ATOM	1933	N	GLN B	64		325 1.00 31.10 B
						752 1.00 30.99 B
ATOM	1934	CA	GLN B	64		
MOTA	1935	CB	GLN B	64		446 1.00 32.54 B
MOTA	1936	CG	GLN B	64	36.988 -24.557 18.	383 1.00 34.49 B
ATOM	1937	CD	GLN B	64	36.870 -25.998 18.	810 1.00 38.20 B
ATOM	1938		GLN B	64	36.629 -26.884 17.	984 1.00 40.82 B
		NE2	GLN B	64		108 1.00 38.34 B
ATOM	1939					
MOTA	1940	C	GLN B	64		
MOTA	1941	0	GLN B	64	33.252 -22.549 18.	064 1.00 29.28 B
ATOM	1942	N	LYS B	65	32.101 -24.476 17.	979 1.00 28.74 B
ATOM	1943	CA	LYS B	65	30.815 -23.812 18.	123 1.00 29.18 B
ATOM	1944	CB	LYS B	65		132 1.00 30.63 B
						_
MOTA	1945	CG	LYS B	65		
ATOM	1946	CD	LYS B	65	29.371 -24.654 15.	.629 1.00 34.44 B
ATOM	1947	CE	LYS B	65	29.688 -25.327 14.	.284 1.00 37.24 B
ATOM	1948	NZ	LYS B	65	29.430 -24.427 13.	109 1.00 37.89 B
			LYS B	65		352 1.00 28.19 B
MOTA	1949	C				
MOTA	1950	0	LYS B	65		
ATOM	1951	N	ASP B	66		.417 1.00 27.58 B
MOTA	1952	CA.	ASP B	66	31.460 -22.504 21.	.636 1.00 27.41 B
MOTA	1953	CB	ASP B	66	32.283 -23.208 22.	.727 1.00 28.45 B
MOTA	1954	CG	ASP B	66	33.559 -23.847 22	.184 1.00 32.24 B
						.183 1.00 33.17 B
MOTA	1955		ASP B	66		
MOTA	1956	OD2	ASP B	66		.765 1.00 33.25 B
MOTA	1957	C	ASP B	66	32.050 -21.131 21	.316 1.00 26.63 B
MOTA	1958	0	ASP B	66	31.468 -20.102 21	.662 1.00 24.32 B
ATOM	1959	N	ILE B	67	33.198 -21.116 20	.640 1.00 26.12 B
			ILE B	67		.273 1.00 26.42 B
ATOM	1960	CA				
MOTA	1961	CB	ILE B	67		
ATOM	1962	CG2	ILE B	67	* *	.290 1.00 28.54 B
MOTA	1963	CG1	ILE B	67	36.094 -20.925 20	.535 1.00 28.25 B
ATOM	1964	CD1	ILE B	67	36.319 -20.321 21	.906 1.00 32.66 B
ATOM	1965	c	ILE B			.300 1.00 26.36 B
						.491 1.00 25.33 B
MOTA	1966	0	ILE B	67		
MOTA	1967	N	LEU B			.261 1.00 26.11 B
ATOM	1968	CA	LEU B	68	31.617 -19.086 17	.267 1.00 26.66 B
MOTA	1969	CB	LEU B	68	31.132 -20.102 16	.235 1.00 27.61 B
ATOM	1970	CG	LEU B	68	31.807 -20.171 14	.872 1.00 30.12 B
			LEU B			.031 1.00 33.09 B
ATOM	1971				31.001 22.220 21	.190 1.00 30.01 B
MOTA	1972		LEU B			
ATOM	1973	C	LEO B			.878 1.00 26.81 B
ATOM	1974	0	LEU B	68	30.067 -17.280 17	.541 1.00 26.19 B
ATOM	1975	N	GLU B	69	29.706 -19.135 18	.756 1.00 28.87 B
ATOM	1976	CA	GLU B		28.509 -18.614 19	.404 1.00 31.55 B
			GLU E			.382 1.00 35.75 B
MOTA	1977	CB				
MOTA	1978	CG	GLU P			
MOTA	1979	œ	GLU E	69	_ <del>-</del>	.673 1.00 47.92 B
MOTA	1980	OE:	L GLU E	69	27.756 -22.454 21	.418 1.00 49.27 B
MOTA	1981	OE:	GLU E			.694 1.00 50.44 B
		C	GLU E			.130 1.00 29.82 B
MOTA	1982					.027 1.00 27.91 B
MOTA	1983	0	GLU E			
MOTA	1984	N	ARG E			.855 1.00 29.32 B
ATOM	1985	CA	ARG E	3 70		.597 1.00 28.97 B
	1986	CB	ARG F	3 70	31.347 -16.315 22	.606 1.00 28.94 B
ATOM			ARG E			.673 1.00 30.55 B
ATOM		L.L.		- <del>-</del>		
ATOM	1987	CG		3 70		.371 1.00 32.35 B
ATOM ATOM	1987 1988	CD	ARG I			.371 1.00 32.35 B
MOTA MOTA MOTA	1987 1988 1989	CD NE	ARG I	3 70	32.040 -19.037 25	.117 1.00 34.83 B
ATOM ATOM	1987 1988	CD NE CZ	ARG I	3 70 3 70	32.040 -19.037 25 32.946 -19.997 25	.117 1.00 34.83 B
MOTA MOTA MOTA	1987 1988 1989	CD NE CZ	ARG I	3 70 3 70	32.040 -19.037 25 32.946 -19.997 25 34.131 -19.875 24	.117 1.00 34.83 B .232 1.00 34.98 B .647 1.00 35.03 B
MOTA MOTA MOTA MOTA	1987 1988 1989 1990 1991	CD NE CZ NH:	ARG I ARG I ARG I 1 ARG I	3 70 3 70 3 70	32.040 -19.037 25 32.946 -19.997 25 34.131 -19.875 24	.117 1.00 34.83 B
MOTA MOTA MOTA	1987 1988 1989 1990	CD NE CZ NH:	ARG I	3 70 3 70 3 70 3 70	32.040 -19.037 25 32.946 -19.997 25 34.131 -19.875 24 32.662 -21.083 25	.117 1.00 34.83 B .232 1.00 34.98 B .647 1.00 35.03 B

ATOM	1994	0	ARG	В	70	30.412	-13.725	20.951	1.00 26.95	В
ATOM	1995	N	LYS		71	31.395		19.608	1.00 25.97	В
ATOM	1996	CA	LYS		71	31.885	-14.236	18.670	1.00 25.98	В
MOTA	1997	CB	Lys	В	71	32.830	-14.877	17.652	1.00 27.62	В
ATOM	1998	CG	LYS	В	71	33.728		16.924	1.00 29.24	В
ATOM	1999	CD	LYS		71	34.628		17.909	1.00 32.14	В
ATOM	2000	CE	LYS		71	35.430		17.236	1.00 33.13	B B
ATOM	2001	NZ	LYS		71	36.093		18.245	1.00 34.18 1.00 25.22	В
ATOM	2002	C	LYS		71	30.710		17.952 17.671	1.00 25.22	В
ATOM	2003	0	LYS		71	30.719 29.701		17.657	1.00 25.08	В
ATOM	2004	N	ARG		72 72	28.500		16.989	1.00 26.32	В
MOTA	2005 2006	CA CB	ARG		72		-15.101	16.561	1.00 28.02	В
MOTA MOTA	2007	CG	ARG		72		-15.830	15.340	1.00 28.10	В
ATOM	2008	CD	ARG		72	27.225		15.083	1.00 32.02	В
ATOM	2009	NE	ARG		72		-17.583	13.766	1.00 36.46	В
ATOM	2010	CZ	ARG		72	27.014	-18.779	13.389	1.00 38.62	В
ATOM	2011		ARG		72	26.324	-19.538	14.238	1.00 37.88	В
ATOM	2012	NH2	ARG	В	72	27.270	-19.212	12.163	1.00 38.55	В
ATOM	2013	С	ARG	В	72		-13.017	17.898	1.00 24.31	В
ATOM	2014	0	ARG	В	72		-12.326	17.439	1.00 24.84	В
MOTA	2015	N	ALA		73		-13.028	19.189	1.00 26.18	B B
MOTA	2016	CA	ALA		73		-12.185	20.140	1.00 28.18 1.00 28.97	В
MOTA	2017	CB	ALA		73		-12.974	21.418 20.472	1.00 28.97	В
ATOM	2018	C	ALA		73	28.056	-10.916 -9.977	21.066	1.00 30.50	В
ATOM	2019	0	ALA ALA		73 74		-10.882	20.070	1.00 29.65	В
ATOM	2020	N CA	ALA		74 74	30.170	-9.732	20.347	1.00 30.77	В
ATOM ATOM	2021 2022	CB	ALA		74	31.558	-9.966	19.764	1.00 30.77	В
ATOM	2023	c	ALA		74	29.594	-8.414	19.827	1.00 31.78	В
ATOM	2024	ŏ	ALA		74	29.789	-7.359	20.438	1.00 32.74	В
ATOM	2025	N	VAL		75	28.886	-8.465	18.704	1.00 31.60	В
ATOM	2026	CA	VAL	В	75	28.308	-7.248	18.145	1.00 32.38	В
ATOM	2027	CB	VAL	В	75	27.397	-7.539	16.929	1.00 30.51	В
MOTA	2028	CG1	. VAI	В	75	27.291	-6.295	16.062	1.00 31.44	В
MOTA	2029	CG2	VAI		75	27.931	-8.696	16.137	1.00 33.08	В
MOTA	2030	С	VAI		75	27.465	-6.529	19.201	1.00 33.07	B B
MOTA	2031	0	VAI		75	27.402	-5.302	19.218	1.00 33.54 1.00 34.70	В
MOTA	2032	N	ASI		76	26.811	-7.302	20.065 21.130	1.00 36.27	В
ATOM	2033	CA	ASI		76 76	25.971 24.780	-6.748 -7.670	21.420	1.00 38.57	В
ATOM	2034	CB	ASI		76 76	23.889	-7.881	20.215	1.00 41.48	В
MOTA MOTA	2035 2036	CG	ASI		76	23.335	-6.887	19.694	1.00 43.46	В
ATOM	2037		ASI		76	23.739	-9.048	19.792	1.00 43.76	В
ATOM	2038	C	ASI		76	26.780	-6.600	22.411	1.00 35.56	В
MOTA	2039	ō	ASI		76	26.731	-5.569	23.081	1.00 34.13	В
ATOM	2040	N	ARC	з в	77	27.508	-7.661	22.744	1.00 35.22	В
MOTA	2041	CA	AR	з в	77	28.343		23.937	1.00 34.49	В
ATOM	2042	CB		3 B	77	29.071		23.991	1.00 37.16	В
ATOM	2043	CG		3 B	77	29.841		25.271	1.00 40.90 1.00 43.79	B B
MOTA	2044	œ		G B	77		-10.553	25.102 24.665	1.00 48.65	В
MOTA	2045	NE		G B	77		-11.743 -12.385	25.406	1.00 51.36	В
MOTA	2046 2047	CZ	AR L AR	GB			-11.949	26.626	1.00 52.34	В
MOTA MOTA	2047		2 AR				-13.470	24.935	1.00 50.76	В
MOTA	2049	C		GВ		29.362		23.927	1.00 32.18	В
ATOM	2050	ō		GВ		29.499		24.896	1.00 32.49	В
ATOM	2051	N		ьв		30.073	-6.442	22.818	1.00 30.66	В
ATOM	2052	CA	VA	ьв	78	31.086		22.707	1.00 29.00	В
MOTA	2053	CB		L B		32.276		21.867	1.00 27.82	В
MOTA	2054		1 VA			33.327			1.00 25.08	B B
ATOM	2055		2 VA			32.870			1.00 23.27 1.00 29.33	В
MOTA	2056			T B		30.594				B
MOTA	2057			TB		30.435 30.354			1.00 28.42	В
MOTA	2058			s b s b		29.927			1.00 29.14	В
MOTA	2059 2060			SE		28.724				В
ATOM ATOM	2060			SE		28.883				В
MOTA	2062			SE		29.679				В
MOTA	2063			s E		31.05				В
ATOM	2064			RG E		27.52	7 -2.693			В
ATOM	2065			RG E		26.34				В
MOTA	2066			RG E		25.07				В
MOTA	2067	CG	AF	RG E	80	24.61	2 -2.973	19.474	1.00 35.65	В

MOTA	2068	CD	ARG	В	80	23.120	-3.273	19.387	1.00 36.01	В
ATOM	2069	NE	ARG	В	80	22.649	-3.243	18.005	1.00 35.49	В
ATOM	2070	CZ	ARG		80	22.913	-4.188	17.108	1.00 37.80	В
ATOM	2071		ARG		80	23.640	-5.242	17.449	1.00 40.57	В
			ARG		80	22.467	-4.075	15.864	1.00 38.86	В
ATOM	2072								1.00 31.24	В
ATOM	2073	C	ARG		80	26.507	-1.552	22.524		
MOTA	2074	0	ARG		80	25.975	-0.525	22.944	1.00 32.07	В
ATOM	2075	N	HIS	В	81	27.257	-2.337	23.283	1.00 31.40	В
ATOM	2076	CA	HIS	В	81	27.492	-2.028	24.683	1.00 32.20	В
MOTA	2077	ÇВ	HIS	В	81	28.220	-3.185	25.366	1.00 33.00	В
ATOM	2078	CG	HIS		81	28.595	-2.899	26.787	1.00 37.24	В
			HIS		81	29.764	-2.490	27.335	1.00 38.05	В
ATOM	2079							27.826	1.00 39.11	В
ATOM	2080		HIS		81	27.692	-2.981			
MOTA	2081		HIS		81	28.290	-2.635	28.952	1.00 40.49	В
MOTA	2082	NE2	HIS	В	81	29.548	-2.332	28.682	1.00 39.16	В
MOTA	2083	C	HIS	В	81	28.326	-0.762	24.831	1.00 30.87	В
ATOM	2084	0	HIS	В	81	27.906	0.206	25.470	1.00 31.38	В
ATOM	2085	N	ASN		82	29.511	-0.770	24.233	1.00 29.77	В
ATOM	2086	CA	ASN		82	30.403	0.375	24.332	1.00 28.02	B
						31.755	0.056	23.683	1.00 26.64	В
ATOM	2087	CB	ASN		82				1.00 25.02	В
ATOM	2088	CG	ASN		82	32.470	-1.092	24.373		
MOTA	2089		asn		82	32.305	-1.305	25.572	1.00 24.06	В
ATOM	2090	ND2	ASN	В	82	33.278	-1.829	23.619	1.00 26.38	В
ATOM	2091	C	ASN	В	82	29.819	1.648	23.741	1.00 26.04	В
MOTA	2092	0	ASN	В	82	30.163	2.747	24.174	1.00 25.71	В
ATOM	2093	N	TYR		83	28.930	1.512	22.765	1.00 25.90	В
			TYR		83	28.324	2.693	22.156	1.00 25.91	В
MOTA	2094	CA						20.946	1.00 25.69	В
MOTA	2095	CB	TYR		83	27.462	2.297			
MOTA	- 2096	CG	TYR	В	83	27.102	3.462	20.056	1.00 25.95	В
ATOM	2097	CD1	TYR	В	83	26.022	4.294	20.353	1.00 27.11	В
MOTA	2098	CE1	TYR	В	83	25.712	5.403	19.545	1.00 25.98	В
MOTA	2099		TYR		83	27.865	3.759	18.933	1.00 27.72	В
ATOM	2100	CE2			83	27.567	4.862	18.121	1.00 28.05	В
					83	26.493	5.680	18.434	1.00 27.73	В
MOTA	2101	CZ	TYR						1.00 27.55	В
MOTA	2102	OH	TYR		83	26.225	6.781	17.645		
ATOM	2103	С	TYR	В	83	27.485	3.458	23.181	1.00 25.87	В
ATOM	2104	0	TYR	В	83	27.315	4.673	23.070	1.00 26.05	В
MOTA	2105	N	GLN	В	84	26.975	2.750	24.186	1.00 28.25	В
ATOM	2106	CA	GLN		84	26.159	3.375	25.229	1.00 30.44	В
	2107	СВ	GLN		84	25.467	2.310	26.093	1.00 34.30	В
MOTA					84	24.595	1.343	25.301	1.00 40.52	В
MOTA	2108	CG	GLN					24.496	1.00 43.21	В
MOTA	2109	CD	GLN		84	23.515	2.047			В
ATOM	2110		. GLN		84	23.023	1.516	23.499	1.00 46.12	
ATOM	2111	NE2	GLN	В	84	23.133	3.244	24.932	1.00 45.41	В
MOTA	2112	С	GLN	В	84	27.030	4.254	26.111	1.00 29.01	В
MOTA	2113	0	GLN	В	84	26.633	5.353	26.494	1.00 27.82	В
ATOM	2114	N	LEU		85	28.219	3.757	26.436	1.00 28.32	В
	2115	CA	LEU		85	29,150	4.505	27.263	1.00 28.76	В
MOTA							3.631	27.631	1.00 28.92	В
MOTA	2116	CB	LEU		85	30.355				В
MOTA	2117	CG	LEU		85	30.065	2.226	28.184	1.00 30.98	
ATOM	2118	CD	LEU	В	85	31.343	1.631	28.758	1.00 30.59	В
MOTA	2119	CD2	LEU	В	85	29.006	2.291	29.265	1.00 31.87	В
MOTA	2120	C	LEU	В	85	29.609	5.719	26.461	1.00 29.95	В
ATOM	2121	0	LEU		85	29.836	6.798	27.010	1.00 30.93	В
ATOM	2122	N	GLU		86	29.724	5.529	25.150	1.00 30.31	В
			GLU		86	30.160	6.577	24.245	1.00 31.41	В
MOTA	2123	CA					5.981	22.861	1.00 32.60	В
MOTA	2124	CB	· GLU		86	30.426				В
MOTA	2125	CG	GL		86	31.741	6.420	22.236	1.00 39.25	
ATOM	2126	CD	GLU	JВ	86	32.962	5.854	22.953	1.00 41.02	В
MOTA	2127	OE:	L GL	JВ	86	33.379	4.714	22.636	1.00 40.75	В
ATOM	2128		2 GLT		86	33.497	6.553	23.843	1.00 41.96	В
MOTA	2129	C	GLU		86	29.113	7.684	24.146	1.00 32.44	В
						29.454	8.865	24.109	1.00 30.73	В
MOTA	2130	0	GL						1.00 33.77	В
MOTA	2131	N	LEU			27.838	7.303	24.103		
MOTA	2132	CA	LE			26.755	8.282	24.015	1.00 34.65	В
MOTA	2133	CB	LE	JB	87	25.398	7.583	23.899	1.00 34.69	В
ATOM	2134	CG	LE	JВ	87	24.916	7.169	22.508	1.00 36.86	В
ATOM	2135		1 LEV			23.655	6.326	22.642	1.00 35.43	В
ATOM	2136		2 LE			24.645		21.660	1.00 35.76	В
	2137			JB		26.740		25.231	1.00 35.16	В
MOTA								25.164	1.00 34.29	В
MOTA	2138			J B		26.250 27.280		26.343	1.00 36.69	В
MOTA	7170	1.7				27 280	× 711	40.343	1.00 30.03	
	2139		AR							
MOTA	2140 2141	CA	AR	G E	88	27.317 27.173	9.493	27.573 28.791	1.00 37.64 1.00 39.79	B

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ATOM	2142	CG	ARG	В	88	25.827	7.878	28.908	1.00 45.19	В
ATOM	2143	CD	ARG	В	88	25.704	7.173	30.253	1.00 49.04	В
ATOM	2144	NE	ARG	В	88	26.657	6.074	30.388	1.00 54.57	В
ATOM	2145	CZ	ARG		88	27.101	5.603	31.552	1.00 55.76	В
			-			26.683	6.137	32.694	1.00 55.56	В
ATOM	2146		ARG		88					
MOTA	2147	NH2	ARG	В	88	27.963	4.595	31.574	1.00 56.11	В
MOTA	2148	C	ARG	В	88	28.601	10.299	27.714	1.00 36.93	В
ATOM	2149	0	ARG	В	88	28.702	11.160	28.589	1.00 37.24	В
ATOM	2150	N	THR	В	89	29.571	10.035	26.842	1.00 35.19	В
		CA	THR		89	30.860	10.712	26.914	1.00 31.71	В
MOTA	2151								1.00 31.61	В
ATOM	2152	CB	THR		89	31.916	9.767	27.529		
ATOM	2153	OG1	THR	В	89	31.980	8.554	26.762	1.00 29.72	В
ATOM	2154	CG2	THR	В	89	31.557	9.436	28.963	1.00 25.87	В
ATOM	2155	C	THR	В	89	31.420	11.254	25.600	1.00 31.31	В
ATOM	2156	ō	THR		89	31.214	12.415	25.249	1.00 32.41	В
			THR		90	32.139	10.403	24.880	1.00 30.72	В
ATOM	2157	N							1.00 30.43	В
MOTA	2158	CA	THR		90	32.766	10.786	23.623		
ATOM	2159	СВ	THR	В	90	33.368	9.558	22.925	1.00 30.54	В
ATOM	2160	OG1	THR	В	90	34.297	8.919	23.808	1.00 33.70	В
ATOM	2161	CG2	THR	В	90	34.099	9.970	21.666	1.00 31.65	В
ATOM	2162	c	THR		90	31.874	11.512	22.625	1,00 30.61	. в
						32.267	12.543	22.070	1.00 30.24	В
MOTA	2163	0	THR		90					В
MOTA	2164	N	TRO		91	30.683	10.977	22.385	1.00 30.30	
MOTA	2165	CA	LEU	В	91	29.767	11.581	21.425	1.00 31.93	В
MOTA	2166	CB	LEU	В	91	28.709	10.554	21.007	1.00 32.55	В
ATOM	2167	CG	LEU		91	29.268	9.315	20.292	1.00 33.01	В
			LEU		91	28.201	8.233	20.205	1.00 33.73	В
MOTA	2168								1.00 31.26	В
MOTA	2169		LEU		91	29.761	9.700	18.902		
ATOM	2170	С	LEU	В	91	29.096	12.872	21.907	1.00 32.38	В
MOTA	2171	0	LEU	В	91	28.402	13.534	21.139	1.00 32.08	В
ATOM	2172	N	GLN	В	92	29.303	13.229	23.173	1.00 32.44	В
MOTA	2173	CA	GLN		92	28.725	14.454	23.713	1.00 34.54	В
						28.138	14.217	25.110	1.00 38.48	В
ATOM	2174	CB	GLN		92					В
MOTA	2175	CG	GLN		92	26.836	13.419	25.121	1.00 44.66	
MOTA	2176	CD	GIM	В	92	26.233	13.291	26.516	1.00 49.27	В
MOTA	2177	OE1	GLN	В	92	25.239	12.588	26.712	1.00 51.65	В
ATOM	2178	NE2	GLN	В	92	26.832	13.975	27.491	1.00 49.93	В
	2179	C	GLN		92	29.779	15.557	23.777	1.00 32.86	' В
MOTA							16.721	24.019	1.00 32.19	В
MOTA	2180	0	GLN		92	29.457				В
ATOM	2181	N	ARG	В	93	31.038	15.187	23.555	1.00 31.53	
MOTA	2182	CA	ARG	В	93	32.132	16.157	23.576	1.00 29.87	В
MOTA	2183	CB	ARG	В	93	33.477	15.472	23.302	1.00 28.14	В
ATOM	2184	CG	ARG	В	93	34.681	16.433	23.217	1.00 23.56	В
	2185	æ	ARG		93	35.953	15.656	22.925	1.00 22.53	В
ATOM							16.486	22.662	1.00 19.19	В
ATOM	2186	NE	ARG		93	37.128			1.00 18.66	В
MOTA	2187	CZ	ARG		93	37.769	17.205	23.581		
ATOM	2188	NHI	. ARG	В	93	37.352	17.214	24.843	1.00 17.45	В
ATOM	2189	NH2	2 ARG	В	93	38.847	17.898	23.242	1.00 16.56	В
MOTA	2190	C	ARG	В	93	31.921	17.245	22.535	1.00 29.02	В
ATOM	2191	ō	ARG		93	31.755	16.965	21.349	1.00 29.55	В
			ARG		94	31.933	18.490	22.987	1.00 28.71	В
MOTA	2192	Ŋ						22.087	1.00 29.63	В
MOTA	2193	CA	ARG		94	31.767	19.613			
ATOM	2194	CB	ARG	B	94	30.299	20.046	22.041	1.00 32.44	В
ATOM	2195	CG	ARG	В	94	29.506	19.196	21.060	1.00 37.10	В
ATOM	2196	CD	ARC	В	94	28.016	19.414	21.124	1.00 39.80	В
ATOM	2197	NE	ARG	B	94	27.350	18.742	20.008	1.00 44.04	В
	2198	CZ	ARG		94	27.372	17.428	19.791	1.00 44.11	В
MOTA							16.625	20.617	1.00 45.60	В
ATOM	2199	NH:			94	28.026				В
MOTA	2200	NH:	2 ARC	3 B	94	26.747	16.916	18.739	1.00 44.45	
ATOM	2201	С	ARC	3 B	94	32.656	20.760	. 22.498	1.00 28.84	В
MOTA	2202	0	ARC	3 B	94	32.464	21.363	23.550	1.00 29.13	В
ATOM	2203	N	VAI		95	33.650	21.038	21.663	1.00 27.49	В
ATOM		CA			95	34.592	22.117	21.916	1.00 26.47	В
	2204					36.047	21.605	21.890	1.00 25.65	В
MOTA	2205	CB		ьв	95				1.00 22.82	В
MOTA	2206	CG:			95	37.004	22.734	22.260		
ATOM	2207	CG	2 VAI	LВ	95	36.202	20.423	22.849	1.00 26.01	В
ATOM	2208	C	VA	LВ	95	34.415	23.180	20.840	1.00 27.00	В
MOTA	2209			L B		34.721	22.945	19.665	1.00 27.00	В
MOTA	2210			UΒ		33.912	24.340	21.253	1.00 26.94	В
						33.673	25.462	20.348	1.00 26.50	В
MOTA	2211			U B					1.00 29.19	В
MOTA	2212			υB		33.072	26.649	21.107		
ATOM	2213			UB		31.736	26.372	21.775	1.00 36.47	В
MOTA	2214	CD	GT.	U B	96	31.211	27.582	22.537	1.00 40.45	В
ATOM	2215		1 GL			30.121	27.477	23.144	1.00 42.85	В

MOTA	2216	OE2	GLU :	В	96	31.891	28.634	22.526	1.00	40.11	В
MOTA	2217	C	GLU :	В	96	34.960	25.916	19.689	1.00	25.02	В
ATOM	2218	0	GLU :	В	96	35.999	26.022	20.338	1.00	24.73	В
ATOM	2219	N	PRO	В	97	34.900	26.204	18.383	1.00	24.54	В
ATOM	2220	CD	PRO		97	33.744	26.011	17.493	1.00	22.89	В
ATOM	2221	CA	PRO		97	36.069	26.655	17.626	1.00	23.87	В
ATOM	2222	СВ	PRO		97	35.580	26.633	16.175		22.81	В
ATOM	2223	CG	PRO		97	34.411	25.663	16.202		25.55	В
					97	36.498	28.061	18.021		23.80	В
ATOM	2224	C	PRO							24.40	В
ATOM	2225	0	PRO		97	35.665	28.905	18.353			
MOTA	2226	N	THR		98	37.799	28.307	17.990		22.02	В
ATOM	2227	CA	THR		98	38.306	29.634	18.266		24.00	В
ATOM	2228	CB	THR	В	98	39.569	29.592	19.150		27.31	В
MOTA	2229	OG1	THR	В	98	40.626	28.929	18.449	1.00	35.69	В
ATOM	2230	CG2	THR	В	98	39.282	28.839	20.439	1.00	26.76	В
ATOM	2231	С	THR	В	98	38.631	30.143	16.860	1.00	22.38	В
ATOM	2232	0	THR	В	98	39.376	29.504	16.116	1.00	19.48	В
MOTA	2233	N	VAL		99	38.041	31.274	16.487	1.00	21.55	В
ATOM	2234	CA	VAL		99	38.242	31.824	15.152	1.00	21.20	В
ATOM	2235	СВ	VAL		99	36.871	32.153	14.509		21.09	В
			VAL		99	37.043	32.541	13.050		19.62	В
ATOM	2236		VAL		99	35.950	30.944	14.625		18.29	В
ATOM	2237	CG2								21.59	В
ATOM	2238	C	VAL		99	39.140	33.059	15.167			
ATOM	2239	0	VAL		99	38.970	33.962	15.982		21.57	В
ATOM	2240	N	THR			40.099	33.084	14.252		22.65	В
MOTA	2241	CA	THR	в:	100	41.056	34.179	14.168		24.95	В
MOTA	2242	CB	THR	в:	100	42.399	33.770	14.820	1.00	26.31	В
MOTA	2243	OG1	THR	B 3	100.	42.162	33.321	16.160	1.00	30.10	В
MOTA	2244	CG2	THR	B :	100	43.359	34.942	14.854	1.00	29.07	В
ATOM	2245	C	THR	в:	100	41.329	34.556	12.717	1.00	24.61	В
ATOM	2246	0	THR	в:	100	41.514	33.689	11.869	1.00	23.89	В
MOTA	2247	N	ILE			41.363	35.852	12.435	1.00	26.18	В
MOTA	2248	CA	ILE			41.638	36.315	11,080		29.32	В
		CB	ILE			40.572	37.327	10.582		29.37	В
MOTA	2249						37.885	9.231		29.49	В
ATOM	2250	CG2				40.986		10.492		30.11	В
ATOM	2251	CG1				39.198	36.664				В
MOTA	2252		ILE			38.110	37.605	10.002		29.81	
ATOM	2253	C	ILE			42.988	37.015	11.040		31.04	В
ATOM	2254	0	ILE	В:	101	43.270	37.868	11.877		31.24	В
MOTA	2255	N	SER	В	102	43.820	36.664	10.066		34.47	В
MOTA	2256	CA	SER	В	102	45.124	37.303	9.940		39.17	В
ATOM	2257	CB	SER	В	102	46.143	36.617	10.844	1.00	37.33	В
MOTA	2258	OG	SER	B :	102	46.326	35.265	10.462	1.00	41.93	В
ATOM	2259	С	SER	В	102	45.632	37.289	8.501	1.00	42.45	В
ATOM	2260	0	SER	В	102	45.641	36.248	7.845	1.00	42.45	В
MOTA	2261	N	PRO	В	103	46.052	38.455	7.988	1.00	45.38	В
ATOM	2262	CD	PRO			45.938	39.793	8.596	1.00	45.47	В
ATOM	2263	CA	PRO			46.564	38.545	6.617	1.00	48.91	В
ATOM	2264	СВ	PRO			46.446	40.032	6.312	1.00	47.74	В
		CG	PRO			46.739	40.652	7.642		47.08	В
MOTA	2265	C	PRO			48.010	38.042	6.545		51.96	В
ATOM	2266						37.957	7.568		52.51	В
MOTA	2267	0	PRO			48.688 48.475	37.699	5.346		55.84	В
MOTA	2268	N	SER				37.209	5.177		60.00	В
MOTA	2269	CA	SER			49.843				59.60	В
MOTA	2270	CB	SER			50.018	36.578	3.791			В
MOTA	2271	OG	SER			49.778	37.520	2.759		59.05	
MOTA	2272	C	SER			50.842	38.353	5.368		63.75	В
MOTA	2273	0	SER			50.853	39.325	4.605		64.64	В
MOTA	2274	N	ARG	В	105	51.677	38.228	6.398		66.99	В
ATOM	2275	CA	ARG	В	105	52.674	39.242	6.736		69.17	В
MOTA	2276	CB	ARG	В	105	53.631	38.700	7.808		70.33	В
MOTA	2277	CG	ARG	В	105	54.672	37.690	7.318		72.24	В
ATOM	2278	CD	ARG	В	105	54.073	36.586	6.449	1.00	73.51	В
MOTA	2279	NE			105	52.981	35.859	7.095	1.00	75.02	В
ATOM	2280	CZ			105	53.120	35.051	8.142	1.00	76.07	В
ATOM	2281		LARG			54.314	34.852	8.684	1.00	77.38	В
ATOM	2282	NH				52.059		8.644		76.05	В
ATOM	2283	C			105	53.464	39.720	5.523		70.38	В
					105	53.134	40.746	4.923		71.56	В
MOTA	2284	0				46.629		-1.867		49.25	В
MOTA	2285	N			113	46.029		-0.515		48.42	В
MOTA	2286	CA			113			0.477		51.23	В
MOTA	2287	CB			113	46.726		1.863		53.89	В
MOTA	2288	CG			113	47.268				55.14	В
ATOM	2289	OD:	1 ASN	В	113	48.429	40.498	2.019	1.00	JJ.14	

MOTA	2290	ND2	asn b	113	46.428	41.048	2.880	1.00 55.30	B
MOTA	2291	C	ASN B	113	46.143	38.808	-0.118	1.00 45.78	В
MOTA	2292	0	ASN B.	113	45.155	38.471	-0.774	1.00 44.99	В
MOTA	2293	N	LEU B	114	46.550	38.146	0.961	1.00 42.27	В
ATOM	2294	CA	LEU B		45.862	36.944	1.415	1.00 38.77	В
ATOM	2295	СВ	LEU B		46.770	35.739	1.182	1.00 39.10	В
ATOM	2296	CG	LEU B		46.238	34.330	1.421	1.00 40.81	В
ATOM	2297		LEU B		45.097	34.023	0.459	1.00 41.59	В
			LEU B		47.379	33.341	1.222	1.00 41.03	В
ATOM	2298					36.986	2.883	1.00 36.39	В
ATOM	2299	C	LEU B		45.424			1.00 35.98	В
ATOM	2300	0	LEU B		46.237	37.204	3.783		
ATOM	2301	И	LEU B		44.130	36.777	3.112	1.00 31.79	В
MOTA	2302	CA	TEA B	115	43.576	36.766	4.460	1.00 28.77	B
MOTA	2303	CB	TEA B	115	42.231	37.496	4.493	1.00 29.52	В
MOTA	2304	CG	LEU B	115	42.156	38.843	5.218	1.00 30.12	В
MOTA	2305	CD1	LEU B	115	43.281	39.751	4.764	1.00 30.28	В
MOTA	2306	CD2	LEU B	115	40.799	39.479	4.951	1.00 28.39	В
ATOM	2307	C	LEU B	115	43.374	35.323	4.896	1.00 27.23	В
ATOM	2308	0	LEU B	115	42.815	34.513	4.154	1.00 25.72	В
ATOM	2309	N	VAL B		43.825	35.002	6.103	1.00 24.13	В
ATOM	2310	CA	VAL B		43.695	33.651	6.618	1.00 20.76	В
ATOM	2311	СВ	VAL B		45.078	33.098	7.078	1.00 20.02	В
			VAL B		44.915	31.757	7.777	1.00 17.46	В
MOTA	2312		VAL B		45.996	32.944	5.880	1.00 19.44	В
MOTA	2313					33.568	7.784	1.00 20.38	В
MOTA	2314	C	VAL B		42.723				В
ATOM	2315	0	VAL B		42.860	34.293	8.766	1.00 19.54	
MOTA	2316	N	CYS B		41.724	32.701	7.669	1.00 20.87	. В
ATOM	2317	CA	CYS B		40.793	32.523	8.774	1.00 22.57	В
ATOM	2318	C	CYS B	117	41.132	31.196	9.444	1.00 21.84	В
MOTA	2319	0	CYS B	117	40.867	30.123	8.892	1.00 22.98	В
MOTA	2320	CB	CYS B	117	39.332	32.486	8.315	1.00 23.53	В
MOTA	2321	SG	CYS B	117	38.217	32.222	9.734	1.00 29.76	В
ATOM	2322	N	SER B	118	41.728	31.277	10.627	1.00 19.87	В
ATOM	2323	CA	SER B	118	42.094	30.092	11.381	1.00 18.65	В
MOTA	2324	СВ	SER B	118	43.345	30.356	12.226	1.00 19.67	В
MOTA	2325	OG	SER B	118	44.463	30.672	11.421	1.00 22.97	В
ATOM	2326	C	SER B	118	40.962	29.656	12.300	1.00 18.03	В
MOTA	2327	0	SER B	118	40.579	30.389	13.209	1.00 19.82	В
ATOM	2328	N	VAL B	119	40.426	28.463	12.050	1.00 17.57	В
ATOM	2329	CA	VAL B	119	39.365	27.889	12.874	1.00 15.30	В
MOTA	2330	СВ	VAL B		38.202	27.364	12.006	1.00 15.69	В
ATOM	2331	CG1	VAL B	119	37.091	26.852	12.892	1.00 11.64	В
ATOM	2332	CG2			37.695	28.484	11.076	1.00 13.82	В
ATOM	2333	C	VAL B		40.073	26.739	13.579	1.00 15.38	В
ATOM	2334	ŏ	VAL B		40.318	25.680	12.992	1.00 16.76	В
ATOM	2335	N	THR B		40.404	26.958	14.844	1.00 16.03	В
ATOM	2336	CA	THR B		41.165	25.988	15.615	1.00 15.04	В
		CB	THR B		42.487	26.613	16.031	1.00 13.75	В
MOTA	2337				42.221	27.713	16.915	1.00 17.84	В
MOTA	2338		. THR B			27.144	14.815	1.00 12.18	В
ATOM	2339		THR B		43.230		16.872	1.00 17.87	В
MOTA	2340	C	THR B		40.533	25.405		1.00 17.71	В
MOTA	2341	0	THR B		39.571	25.944	17.425	1.00 17.71	В
MOTA	2342	N	ASP B		41.132	24.303	17.317		В
ATOM	2343	CA	ASP B		40.738	23.576	18.511	1.00 20.97	
ATOM	2344	CB	ASP B		41.268	24.291	19.766	1.00 24.82	В
MOTA	2345	CG	ASP B	121	42.797	24.330	19.831	1.00 31.04	В
ATOM	2346	OD:	L ASP B	121	43.460	23.360	19.397	1.00 30.81	В
ATOM	2347	OD	ASP B	121	43.339	25.333	20.346	1.00 34.38	В
MOTA	2348	C	ASP B	121	39.238	23.293	18.679	1.00 21.27	В
ATOM	2349	0	ASP B	121	38.629	23.671	19.683	1.00 23.00	В
ATOM	2350	N	PHE B		38.641	22.613	17.710	1.00 20.38	В
ATOM	2351	CA	PHE B		37.233	22.280	17.818	1.00 18.51	В
ATOM	2352	CB	PHE B		36.414	22.988	16.732	1.00 16.18	В
MOTA	2353	CG	PHE B		36.817		15.319	1.00 13.31	В
			PHE B		37.695		14.615	1.00 11.43	В
MOTA	2354		2 PHE E		36.247		14.664	1.00 10.93	В
MOTA	2355				37.998		13.272	1.00 10.91	В
MOTA	2356		1 PHE E		36.541		13.317	1.00 12.31	В
MOTA	2357		2 PHE E		37.419		12.618	1.00 8.92	В
MOTA	2358							1.00 19.55	В
MOTA	2359		PHE E		37.011		17.739	1.00 19.55	В
MOTA	2360		PHE E		37.889		17.301	1.00 18.45	В
ATOM	2361		TYR E		35.829		18.182	1.00 20.50	В
ATOM	2362				35.412		18.180		В
MOTA	2363	CB	TYR I	3 123	36.067	18.201	19.340	1.00 19.11	5

ATOM 2364 CG TYR B 123 35.919 16.702 19.228 1.00 18.56 ATOM 2366 CE1 TYR B 123 34.746 16.062 19.629 1.00 19.13 ATOM 2367 CD2 TYR B 123 34.572 14.695 19.446 1.00 17.75 ATOM 2368 CE2 TYR B 123 36.920 15.932 18.647 1.00 17.20 ATOM 2369 CZ TYR B 123 35.584 13.953 18.853 1.00 19.59 ATOM 2370 OH TYR B 123 35.584 13.953 18.853 1.00 19.59 ATOM 2371 C TYR B 123 35.841 13.953 18.631 1.00 22.32 ATOM 2372 O TYR B 123 33.896 18.957 18.351 1.00 21.83 ATOM 2373 N PRO B 124 33.175 18.126 17.584 1.00 21.65 ATOM 2373 N PRO B 124 33.175 18.126 17.584 1.00 23.26 ATOM 2375 CA PRO B 124 33.627 17.177 16.562 1.00 23.81 ATOM 2377 CG PRO B 124 33.298 16.901 16.56 1.00 23.07 ATOM 2377 CG PRO B 124 33.298 16.901 16.56 1.00 23.07 ATOM 2378 C PRO B 124 34.128 17.813 15.266 1.00 23.07 ATOM 2378 C PRO B 124 34.128 17.813 15.266 1.00 23.07 ATOM 2379 O PRO B 124 34.294 19.035 15.149 1.00 24.43 ATOM 2380 N ALA B 125 34.457 16.971 14.291 1.00 24.43 ATOM 2381 CA ALA B 125 34.457 16.971 14.291 1.00 20.20 ATOM 2382 CB ALA B 125 34.557 18.222 12.078 1.00 22.13 ATOM 2384 O ALA B 125 34.557 18.598 11.407 1.00 24.48 ATOM 2386 CA GLN B 126 30.293 16.595 11.400 1.00 24.48 ATOM 2386 CA GLN B 126 30.293 16.595 11.400 1.00 24.48 ATOM 2389 CD GLN B 126 30.293 16.595 11.400 1.00 24.48 ATOM 2389 CD GLN B 126 30.293 16.595 11.400 1.00 24.48 ATOM 2389 CD GLN B 126 30.293 16.595 11.400 1.00 29.99 ATOM 2389 CD GLN B 126 30.293 16.595 11.400 1.00 29.99 ATOM 2389 CD GLN B 126 30.293 16.595 11.400 1.00 29.99 ATOM 2399 OFL GLN B 126 30.293 16.595 11.400 1.00 29.99 ATOM 2399 CD GLN B 126 30.293 16.595 11.400 1.00 29.36 ATOM 2399 CD GLN B 126 30.293 16.595 11.400 1.00 29.36 ATOM 2399 CD GLN B 126 30.293 16.595 11.400 1.00 29.99 ATOM 2399 CD GLN B 126 30.293 16.595 11.400 1.00 29.99 ATOM 2399 CD GLN B 126 30.293 16.595 11.400 1.00 29.36 ATOM 2399 CD GLN B 126 30.293 16.595 11.400 1.00 29.36 ATOM 2399 CD GLN B 126 30.293 16.595 11.400 1.00 29.36 ATOM 2399 CD GLN B 126 30.293 16.595 11.400 10.00 29.36 ATOM 2399 CD GLN B 126 30.293 10.027 10.023 10.027 10.023 10.023 10.023	888888888888888888888888888888888888888
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ATOM 2403 CA LYS B 128 31.457 24.884 7.689 1.00 27.45	В
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	В
ATOM 2406 CD LYS B 128 30.129 24.954 4.793 1.00 38.25	В
ATOM 2407 CE LYS B 128 29.802 25.742 3.517 1.00 40.20	В
ATOM 2408 NZ LYS B 128 30.281 25.071 2.271 1.00 39.87	В
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ATOM 2416 C VAL B 129 33.248 28.791 5.778 1.00 25.17	B B B
ATOM 2417 O VAL B 129 33.532 28.283 4.701 1.00 25.50	B B B
ATOM 2418 N ARG B 130 32.724 30.007 5.884 1.00 27.21	B B B B
ATOM 2419 CA ARG B 130 32.445 30.814 4.701 1.00 28.49	B B B
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ATOM 2422 CD ARG B 130 28.927 29.813 3.432 1.00 41.30 ATOM 2423 NE ARG B 130 27.834 30.254 4.291 1.00 42.15 ATOM 2424 CZ ARG B 130 27.032 29.426 4.953 1.00 46.05 ATOM 2425 NH1 ARG B 130 27.200 28.112 4.849 1.00 45.50 ATOM 2426 NH2 ARG B 130 26.061 29.910 5.718 1.00 48.30 ATOM 2427 C ARG B 130 33.036 32.211 4.792 1.00 27.57 ATOM 2428 O ARG B 130 33.130 32.789 5.874 1.00 26.00	8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
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ATOM 2422 CD ARG B 130 28.927 29.813 3.432 1.00 41.30 ATOM 2423 NE ARG B 130 27.834 30.254 4.291 1.00 42.15 ATOM 2424 CZ ARG B 130 27.032 29.426 4.953 1.00 46.05 ATOM 2425 NH1 ARG B 130 27.202 28.112 4.849 1.00 45.50 ATOM 2426 NH2 ARG B 130 26.061 29.910 5.718 1.00 48.30 ATOM 2427 C ARG B 130 33.036 32.211 4.792 1.00 27.57 ATOM 2428 O ARG B 130 33.130 32.789 5.874 1.00 26.00 ATOM 2429 N TRP B 131 33.440 32.744 3.645 1.00 27.37 ATOM 2430 CA TRP B 131 34.004 34.085 3.571 1.00 30.27 ATOM 2431 CB TRP B 131 35.281 34.083 2.737 1.00 30.21 ATOM 2432 CG TRP B 131 36.532 33.844 3.521 1.00 32.32 ATOM 2433 CD2 TRP B 131 37.155 34.757 4.432 1.00 32.41	8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
ATOM 2422 CD ARG B 130 28.927 29.813 3.432 1.00 41.30 ATOM 2423 NE ARG B 130 27.834 30.254 4.291 1.00 42.15 ATOM 2424 CZ ARG B 130 27.032 29.426 4.953 1.00 46.05 ATOM 2425 NH1 ARG B 130 27.200 28.112 4.849 1.00 45.50 ATOM 2426 NH2 ARG B 130 26.061 29.910 5.718 1.00 48.30 ATOM 2427 C ARG B 130 33.036 32.211 4.792 1.00 27.57 ATOM 2428 O ARG B 130 33.130 32.789 5.874 1.00 26.00 ATOM 2429 N TRP B 131 33.440 32.744 3.645 1.00 27.37 ATOM 2430 CA TRP B 131 34.004 34.085 3.571 1.00 30.27 ATOM 2431 CB TRP B 131 35.281 34.083 2.737 1.00 30.21 ATOM 2432 CG TRP B 131 36.532 33.844 3.521 1.00 32.32 ATOM 2433 CD2 TRP B 131 37.155 34.757 4.432 1.00 32.41	8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
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					20 102	24 764	5.812	1.00 32.82	В
MOTA	2438		TRP B		39.193	34.764			
MOTA	2439	CZ3	TRP B		37.680	36.656	5.800	1.00 32.08	В
MOTA	2440	CH2	TRP B	131	38.849	36.017	6.249	1.00 33.40	В
ATOM	2441	C	TRP B	131	33.003	35.064	2.949	1.00 32.99	В
MOTA	2442	0	TRP B	131	32.367	34.759	1.940	1.00 32.18	В
ATOM	2443	N	PHE B	132	32.879	36.242	3.550	1.00 35.48	В
MOTA	2444	CA	PHE B		31.962	37.263	3.058	1.00 39.35	В
		СВ	PHE B		30.856	37.501	4.077	1.00 38.14	В
MOTA	2445							1.00 38.39	В
ATOM	2446	CG	PHE B		29.843	36.407	4.123		
ATOM	2447		PHE B		28.804	36.373	3.202	1.00 38.31	В
MOTA	2448	CD2	PHE B	132	29.930	35.399	5.075	1.00 38.21	В
MOTA	2449	CE1	PHE B	132	27.860	35.348	3.229	1.00 39.26	В
MOTA	2450	CE2	PHE B	132	28.992	34.369	5.111	1.00 38.83	В
ATOM	2451	CZ	PHE B		27.954	34.345	4.184	1.00 37.91	В
			PHE B		32.650	38.583	2.755	1.00 41.59	В
ATOM	2452	C					3.508	1.00 42.72	В
ATOM	2453	0	PHE B		33.515	39.025			
ATOM	2454	N	ARG B		32.267	39.203	1.640	1.00 45.04	В
MOTA	2455	CA	ARG B	133	32.829	40.490	1.242	1.00 48.28	В
MOTA	2456	CB	ARG B	133	32.510	40.787	-0.227	1.00 51.68	В
ATOM	2457	CG	ARG B	133	33.293	41.958	-0.829	1.00 55.78	В
ATOM	2458	CD	ARG B		34.787	41.655	-0.867	1.00 57.07	В
ATOM	2459	NE	ARG B		35.580	42.741	-1.440	1.00 59.30	В
						43.135	-2.710	1.00 60.93	В
MOTA	2460	CZ	ARG B		35.523				В
MOTA	2461		ARG B		34.702	42.536	-3.564	1.00 61.44	
ATOM	2462	NH2	ARG B	133	36.295	44.132	-3.128	1.00 61.77	В
MOTA	2463	Ç	ARG B	133	32.129	41.492	2.145	1.00 49.07	В
ATOM	2464	0	ARG E	133	32.299	41.460	3.358	1.00 51.26	В
ATOM	2465	N	ASN E		31.331	42.376	1.572	1.00 49.23	В
ATOM	2466	CA	ASN E		30.614	43.336	2.393	1.00 48.83	В
			ASN E		30.582	44.702	1.710	1.00 45.93	В
ATOM	2467	CB						1.00 45.10	В
MOTA	2468	CG	ASN E		31.973	45.290	1.523		
ATOM	2469		ASN E		32.450	45.440	0.397	1.00 41.81	В
ATOM	2470	ND2	ASN E	134	32.634	45.618	2.634	1.00 41.82	В
ATOM	2471	С	ASN E	134	29.203	42.795	2.594	1.00 50.25	В
ATOM	2472	0	ASN E	134	28.222	43.529	2.508	1.00 52.28	В
ATOM	2473	N	ASP E		29.122	41.496	2.868	1.00 50.15	В
			ASP E		27.847	40.819	3.072	1.00 51.07	В
MOTA	2474	CA						1.00 51.76	В
ATOM	2475	C	ASP E		27.590	39.855	1.910		
MOTA	2476	0	ASP E		26.586	39.136	1.893	1.00 51.82	В
ATOM	2477	N	GLN F	3 136	28.507	39.856	0.944	1.00 50.97	В
ATOM	2478	CA	GLN E	3 136	28.421	38.999	-0.240	1.00 51.24	В
MOTA	2479	CB	GLN E	3 136	28.766	39.805	-1.493	1.00 53.78	В
ATOM	2480	CG	GLN E		28.736	39.000	-2.783	1.00 58.16	В
ATOM		æ	GLN E		29.675	39.559	-3.839	1.00 59.39	В
	2481					39,527	-3.675	1.00 60.12	В
ATOM	2482		GLN E		30.895			1.00 59.45	В
MOTA	2483		GFN E		29.110	40.078	-4.926		
ATOM	2484	C	GLN I		29.395	37.825	-0.124	1.00 49.46	В
MOTA	2485	0	GLN I	3 136	30.607	38.026	-0.035	1.00 48.29	В
MOTA	2486	N	GLU I	3 137	28.873	36.603	-0.144	1.00 47.64	В
MOTA	2487	CA	GLU I	3 137	29.730	35.432	-0.027	1.00 46.85	В
MOTA	2488	CB	GLU F	3 137	28.899	34.152	0.022	1.00 47.17	В
ATOM	2489	CG		3 137	29.695	32.975	0.556	1.00 50.22	В
					28.866	31.726	0.743	1.00 52.65	В
ATOM	2490	CD		3 137				1.00 55.57	В
ATOM	2491		GLU 1		27.699	31.842	1.171	1.00 54.41	В
MOTA	2492		GLU I		29.391	30.623	0.478		
MOTA	2493	С		В 137	30.755	35.320	-1.149	1.00 45.23	В
MOTA	2494	0	GLU I	B 137	30.445	35.544	-2.314	1.00 45.04	В
MOTA	2495	N	GLU I	B 138	31.983	34.977	-0.776	1.00 44.63	В
ATOM	2496	CA		B 138	33.078	34.808	-1.724	1.00 44.36	В
ATOM	2497	СВ		B 138	34.284	35.658	-1.307	1.00 45.65	В
					34.076		-1.320	1.00 48.42	В
MOTA	2498	CG		B 138				1.00 50.71	В
MOTA	2499	CD		B 138	34.144		-2.717		
MOTA	2500	OE1	. GLU	B 138	35.120		-3.442	1.00 51.60	В
ATOM	2501	OE2	GLU :	B 138	33.227	38.526	-3.086	1.00 50.99	В
MOTA	2502	C	GLU	B 138	33.498	33.335	-1.740	1.00 43.68	В
ATOM	2503	ō		B 138	33.831		-0.697	1.00 43.53	В
		N		B 139	33.468		-2.914	1.00 42.58	В
ATOM	2504				33.881		-3.044	1.00 41.76	В
ATOM	2505	CA		B 139				1.00 41.04	В
MOTA	2506	CB		B 139	32.739		-3.543		В
MOTA	2507		L THR		32.207		-4.759	1.00 40.71	
MOTA	2508	CG:	THR	B 139	31.641		-2.492	1.00 41.89	В
ATOM	2509	C	THR	B 139	35.038	31.245	-4.026		В
ATOM	2510	ō		B 139	35.855		-3.981		В
ATOM	2511	N		B 140	35.096		-4.920	1.00 40.67	В
AT ON	w 3 T T	44	- Lun						

MOTA	2512	CA	ALA B	140	36.179	32.305	-5.887	1.00 41.22	В
ATOM	2513	СВ	ALA B	140	35.714	33.016	-7.158	1.00 41.13	В
MOTA	2514	C	ALA B		37.247	33.126	-5.177	1.00 41.09	В
			ALA B		36.976	34.232	-4.693	1.00 43.11	В
MOTA	2515	0							
MOTA	2516	N	GLY B		38.455	32.582	-5.102	1.00 39.60	В
ATOM	2517	CA	GLY B	141	39.526	33.278	-4.418	1.00 35.11	В
ATOM	2518	C	GLY B	141	39.739	32,651	-3.051	1.00 33.42	В
ATOM	2519	0	GLY B	141	40.605	33.076	-2.287	1.00 31.24	В
		N	VAL B		38.945	31.628	-2.750	1.00 31.89	В
ATOM	2520								
MOTA	2521	CA	VAL B		39.033	30.937	-1.470	1.00 32.27	В
MOTA	2522	CB	VAL B	142	37.645	30.790	-0.813	1.00 31.90	В
ATOM	2523	CG1	VAL B	142	37.733	29.861	0.400	1.00 32.37	В
ATOM	2524	CG2	VAL B	142	37.125	32.161	-0.402	1.00 32.53	В
ATOM	2525	C	VAL B		39.652	29.552	-1.564	1.00 31.26	В
			VAL B				-2.343	1.00 32.44	В
ATOM	2526	0			39.211	28.712			
ATOM	2527	N	VAL B		40.676	29.326	-0.752	1.00 30.76	В
MOTA	2528	CA	VAL B	143	41.357	28.045	-0.702	1.00 29.79	В
ATOM	2529	CB	VAL B	143	42.815	28.154	-1.162	1.00 29.63	В
ATOM	2530		VAL B		43.439	26.768	-1.212	1.00 31.60	В
	2531	CG2			42.885	28.819	-2.514	1.00 33.43	В
ATOM									В
ATOM	2532	С	VAL B		41.357	27.575	0.749	1.00 30.61	
MOTA	2533	0	VAL B	143	41.665	28.338	1.667	1.00 28.64	В
ATOM	2534	N	SER B	144	41.017	26.313	0.950	1.00 29.65	В
ATOM	2535	CA	SER B	144	40.970	25.756	2.282	1.00 28.42	В
MOTA	2536	CB	SER B		39.541	25.325	2.605	1.00 29.23	В
			SER B		39.457	24.705	3.875	1.00 33.81	В
MOTA	2537	OG							В
MOTA	2538	C	SER B		41.900	24.562	2.373	1.00 27.32	
ATOM	2539	0	SER B	144	42.101	23.840	1.397	1.00 27.40	В
ATOM	2540	N	THR B	145	42.492	24.372	3.542	1.00 25.70	В
ATOM	2541	CA	THR B	145	43.364	23.227	3.755	1.00 24.82	В
	2542	CB	THR B		44.272	23.418	4.995	1.00 25.01	В
MOTA						23.399	6.186	1.00 25.18	В
ATOM	2543		THR B		43.467				
MOTA	2544	CG2			45.022	24.743	4.923	1.00 23.27	В
MOTA	2545	С	THR B	145	42.392	22.100	4.071	1.00 24.16	В
ATOM	2546	0	THR B	145	41.200	22.335	4.272	1.00 23.86	В
ATOM	2547	N	PRO B	146	42.865	20.854	4.081	1.00 23.17	В
MOTA	2548	CD	PRO B		44.116	20.231	3.618	1.00 22.29	В
						19.852	4.419	1.00 23.18	В
ATOM	2549	CA	PRO B		41.854				
MOTA	2550	CB	PRO B		42.521	18.536	4.008	1.00 24.20	В
MOTA	2551	CG	PRO B	146	43.998	18.833	4.162	1.00 22.82	В
MOTA	2552	С	PRO B	146	41.597	19.945	5.933	1.00 22.63	В
ATOM	2553	0	PRO B	146	42.213	20.766	6.625	1.00 21.32	В
ATOM	2554	N	LEU B		40.667	19.146	6.445	1.00 22.60	В
			LEU B		40.414	19.142	7.883	1.00 22.34	В
ATOM	2555	CA							В
MOTA	2556	CB	TER B		39.241	18.216	8.213	1.00 22.17	
MOTA	2557	CG	TEO B	147	38.934	17.973	9.691	1.00 24.53	В
ATOM	2558	CD1	LEU B	147	38.629	19.288	10.368	1.00 25.95	В
ATOM	2559	CD2	LEU B	147	37.746	17.026	9.826	1.00 25.55	В
ATOM	2560	C	LEU E	147	41.710	18.609	8.515	1.00 21.99	В
			LEU B		42.290	17.640	8.024	1.00 21.35	В
MOTA	2561	0						1.00 20.48	В
MOTA	2562	N	ILE E		42.175	19.246	9.581		
MOTA	2563	CA	ILE E		43.406	18.813	10.228	1.00 19.15	В
MOTA	2564	CB	ILE E	148	44.392	19.990	10.403	1.00 21.68	В
ATOM	2565	CG2	ILE F	148	45.666	19.505	11.065	1.00 20.10	В
MOTA	2566		ILE E		44.728	20.609	9.041	1.00 25.04	В
			ILE		45.416	19.649	8.090	1.00 29.06	В
ATOM	2567							1.00 17.56	В
ATOM	2568	C	ILE E		43.160	18.208	11.603		
MOTA	2569	0	ILE E		42.566	18.852	12.467	1.00 14.88	В
MOTA	2570	N	ARG I	3 149	43.625	16.973	11.795	1.00 15.95	В
MOTA	2571	CA	ARG I	3 149	43.492	16.273	13.077	1.00 17.47	. В
MOTA	2572	CB	ARG E		43.420	14.763	12.852	1.00 16.94	В
ATOM	2573	CG	ARG I		43.202	13.941	14.128	1.00 20.29	В
			ARG I		43.252	12.448	13.821	1.00 21.64	В
MOTA	2574	CD						1.00 21.01	В
MOTA	2575	NE	ARG I		42.168	12.028	12.938		
MOTA	2576	CZ	ARG I		40.934	11.742	13.348	1.00 23.22	В
ATOM	2577	NH:	L ARG I	3 149	40.015	11.374	12.471	1.00 23.89	В
MOTA	2578		2 ARG I		40.623	11.803	14.636	1.00 23.11	В
ATOM	2579	C		B 149	44.720	16.603	13.937	1.00 17.66	В
		ō		B 149	45.850	16.311	13.549	1.00 17.51	В
MOTA	2580				44.496	17.210	15.098	1.00 16.67	В
ATOM	2581	N		B 150				1.00 16.94	В
MOTA	2582	CA		B 150	45.592	17.593	15.980		
MOTA	2583	CB		B 150	45.174	18.756	16.890	1.00 15.38	В
ATOM	2584	CG		B 150	44.899	20.034	16.118	1.00 18.41	В
MOTA	2585		1 ASN	B 150	45.685	20.436	15.249	1.00 19.05	В

ATOM	2586	ND2	ASN B	150	43.790	20.691	16.440	1.00 17.88	В
MOTA	2587	C	ASN B	150	46.116	16.452	16.841	1.00 18.47	В
MOTA	2588	0	asn b	150	47.220	16.540	17.384	1.00 17.03	В
MOTA	2589	N	GLY B		45.324	15.391	16.968	1.00 17.77	В
MOTA	2590	CA	GLY B		45.734	14.251	17.770	1.00 19.16	В
MOTA	2591	C	GLY B		45.258	14.293	19.213	1.00 20.44	В
ATOM	2592	0	GLY B		45.198	13.264	19.877	1.00 22.31 1.00 20.79	B B
ATOM	2593	N CA	ASP B		44.906 44.450	15.475 15.624	19.701 21.077	1.00 20.73	B
ATOM ATOM	2594 2595	CB	ASP B		45.192	16.790	21.748	1.00 21.95	В
ATOM	2596	CG	ASP B		45.027	18.101	20.992	1.00 28.05	В
ATOM	2597		ASP B		45.764	19.060	21.300	1.00 30.94	В
ATOM	2598		ASP B		44.158	18.181	20.090	1.00 28.02	В
ATOM	2599	С	ASP B		42.939	15.847	21.175	1.00 20.51	В
ATOM	2600	0	ASP B	152	42.474	16.619	22.010	1.00 21.63	В
ATOM	2601	N	TRP B	153	42.183	15.166	20.322	1.00 19.19	В
ATOM	2602	CA	TRP B		40.724	15.278	20.300	1.00 16.82	В
ATOM	.2603	CB	TRP B		40.121	14.865	21.657	1.00 15.80	В
MOTA	2604	CG	TRP B		40.326	13.408	22.005	1.00 16.21	В
ATOM	2605		TRP B		39.415	12.322	21.756	1.00 16.58	В
MOTA	2606	CE2			40.047	11.134	22.188 21.211	1.00 15.08 1.00 15.69	B
MOTA	2607	CE3	TRP B		38.125 41.435	12.238 12.848	22.564	1.00 14.68	В
ATOM	2608 2609		TRP B		41.278	11.483	22,677	1.00 15.53	В
MOTA MOTA	2610		TRP B		39.438	9.879	22.087	1.00 15.60	В
ATOM	2611		TRP B		37.518	10.987	21.112	1.00 14.22	В
ATOM	2612		TRP B		38.176	9.827	21.549	1.00 13.89	В
ATOM	2613	C	TRP B	153	40.194	16.660	19.890	1.00 16.09	В
ATOM	2614	0	TRP B	153	39.159	17.110	20.379	1.00 14.28	В
ATOM	2615	N	THR B	154	40.929	17.342	19.020	1.00 15.11	В
ATOM	2616	CA	THR B	154	40.499	18.627	18.483	1.00 16.19	В
MOTA	2617	CB	THR B		41.176	19.877	19.150	1.00 18.02	В
MOTA	2618		THR B		42.602	19.804	19.008	1.00 19.50	В
ATOM	2619	CG2			40.788	20.000	20.608	1.00 15.03 1.00 15.24	B B
ATOM	2620	C	THR B		40.908 41.773	18.602 17.832	17.024 16.635	1.00 15.24	В
ATOM	2621	и О	THR B		40.269	19.437	16.220	1.00 18.04	В
MOTA MOTA	2622 2623	CA	PHE B		40.577	19.538	14.801	1.00 16.03	В
ATOM	2624	CB	PHE B		39.404	19.042	13.938	1.00 16.98	В
ATOM	2625	CG	PHE B		39.069	17.579	14.118	1.00 17.58	В
ATOM	2626	CD1	PHE B		38.133	17.170	15.074	1.00 18.20	В
ATOM	2627	CD2	PHE B	155	39.670	16.611	13.312	1.00 17.71	В
MOTA	2628		PHE B		37.799	15.810	15.223	1.00 17.81	В
ATOM	2629	CE2			39.346	15.250	13.451	1.00 17.57	В
MOTA	2630	CZ	PHE B		38.407	14.849	14.409	1.00 16.39	B B
ATOM	2631	C	PHE B		40.793	21.015 21.870	14.503 15.352	1.00 16.67 1.00 16.84	В
ATOM	2632 2633	N N	PHE B		40.532 41.281	21.312	13.304	1.00 14.72	В
ATOM ATOM	2634	CA	GLN B		41.467	22.689	12.886	1.00 14.66	В
ATOM	2635	СВ	GLN B		42.811	23.264	13.357	1.00 16.69	В
MOTA	2636	CG	GLN B		44.039	22.698	12.669	1.00 15.65	В
ATOM	2637	CD	GLN E	156	45.292	23.486	13.011	1.00 17.87	В
ATOM	2638	OE1	. GLN E	156	45.477	24.617	12.555	1.00 17.56	В
MOTA	2639	NE2	GLN E		46.153	22.897	13.830	1.00 15.40	В
MOTA	2640	C	GLN E		41.398	22.722	11.371	1.00 14.00	В
MOTA	2641	0	GLN E		41.477	21.691	10.716	1.00 15.17	В
ATOM	2642	N	ILE E		41.241	23.911	10.818 9.383	1.00 15.34 1.00 17.26	B B
MOTA	2643	CA	ILE E		41.165 39.791	24.057 23.585	8.856	1.00 17.26	В
MOTA	2644 2645	CB	ILE E		38.675	24.429	9.474	1.00 13.07	В
MOTA MOTA	2646		LILE		39.765	23.649	7.326	1.00 17.72	В
ATOM	2647		LILEE		38.583	22.913	6.712	1.00 14.50	В
ATOM	2648	C	ILE F		41.379	25.523	9.074	1.00 18.67	В
ATOM	2649	0	ILE F	3 157	40.823	26.391	9.745	1.00 22.28	В
MOTA	2650	N	LEU I		42.217	25.795	8.083	1.00 18.98	В
MOTA	2651	CA	LEU I		42.508	27.162	7.690	1.00 20.77	В
MOTA	2652	CB	LEU I		44.022	27.368	7.555	1.00 22.23	В
ATOM	2653	CG	LEU I		44.851	27.525	8.838 9.740	1.00 26.12 1.00 29.01	B B
MOTA	2654		l LEU I 2 LEU I		44.689 46.311	26.320 27.701	8.465	1.00 28.46	В
MOTA MOTA	2655 2656	CD.		B 158	40.311	27.701	6.371	1.00 20.61	В
ATOM	2657	0		B 158	41.934	26.734	5.401	1.00 19.39	В
ATOM	2658	N		B 159	41.088	28.596	6.346	1.00 21.67	В
ATOM	2659	CA	VAL I	B 159	40.380	29.011	5.141	1.00 21.90	В

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ATOM	2660	CB	VAL B	159	38.855	29.061	5.365	1.00 22.06	В
ATOM	2661	CG1	VAL B	159	38.147	29.252	4.043	1.00 20.55	В
			VAL B		38.381	27.766	6.009	1.00 20.83	В
ATOM	2662								
MOTA	2663	C	VAL B	159	40.899	30.379	4.749	1,00 21.80	В
ATOM	2664	0	VAL B	159	40.721	31.357	5.473	1.00 20.82	В
ATOM	2665	N	MET B		41.555	30.416	3.592	1.00 23.56	В
MOTA	2666	CA	MET B	160	42.179	31.613	3.055	1.00 25.12	В
MOTA	2667	CB	MET B	160	43.580	31.257	2.559	1.00 26.80	В
		CG	MET B		44.479	30.736	3.678	1.00 32.00	В
MOTA	2668								
MOTA	2669	SD	MET B	160	45.850	29.700	3.145	1.00 38.02	В
ATOM	2670	CE	MET B	160	45.094	28.065	3.307	1.00 35.43	В
	2671	C	MET B		41.387	32.269	1.941	1.00 28.27	В
MOTA									
ATOM	2672	0	MET B	160	40.684	31.602	1.177	1.00 28.76	В
ATOM	2673	N	LEU B	161	41.518	33.588	1.854	1.00 29.59	В
	2674	CA	LEU B		40.820	34.366	0.845	1.00 32.69	В
ATOM									
ATOM	2675	CB	PEA B	161	39.669	35.142	1.487	1.00 30.80	В
ATOM	2676	CG	LEU B	161	39.031	36.199	0.586	1.00 31.56	В
MOTA	2677	CD1	LEU B	161	38.156	35.516	-0.460	1.00 29.64	В
									В
MOTA	2678		LEU B		38.213	37.167	1.423	1.00 29.89	
ATOM	2679	C	LEU B	161	41.755	35.349	0.154	1.00 35.59	В
ATOM	2680	0	LEU B	161	42.350	36.216	0.801	1.00 35.54	В
						35.203	-1.158	1.00 39.87	В
MOTA	2681	N	GLU B		41.895				
MOTA	2682	CA	GLU B	162	42.728	36.118	-1.927	1.00 44.05	В
ATOM	2683	CB	GLU B	162	42.995	35.565	-3.331	1.00 46.86	В
			GLU B		43.795	36.497	-4.239	1.00 50.98	В
ATOM	2684	CG							
MOTA	2685	CD	GLU B	162	45.274	36.537	-3.891	1.00 54.75	В
ATOM	2686	OE1	GLU B	162	45.604	36.802	-2.715	1.00 56.53	В
		OE2			46.108	36.308	-4.796	1.00 55.16	В
ATOM	2687								
ATOM	2688	C	GLU B	162	41.879	37.372	-2.029	1.00 44.69	В
ATOM	2689	0	GLU B	162	40.719	37.302	-2.434	1.00 44.39	В
		N	MET B		42.436	38.514	-1.648	1.00 46.67	В
MOTA	2690								
ATOM	2691	CA	MET B	163	41.670	39.746	-1.716	1.00 49.56	В
MOTA	2692	CB	MET B	163	40.881	39.949	-0.412	1.00 51.22	В
ATOM	2693	CG	MET B		41.652	39.675	0.876	1.00 51.58	В
									В
MOTA	2694	SD	MET B	163	42.910	40.901	1.274	1.00 56.87	
MOTA	2695	CE	MET B	163	41.915	42.187	2.029	1.00 54.89	В
ATOM	2696	C	MET B	163	42.487	40.986	-2.028	1.00 51.43	В
							-1.942	1.00 51.02	В
ATOM	2697	0	MET B		43.717	40.988			
ATOM	2698	N	THR B	164	41.777	42.038	-2.412	1.00 53.70	В
ATOM	2699	CA	THR B	164	42.385	43.316	-2.738	1.00 56.61	В
			THR B		41.889	43.820	-4.116	1.00 57.48	В
ATOM	2700	CB							
ATOM	2701	OG1	THR E	164	40.457	43.744	-4.172	1.00 57.81	В
MOTA	2702	CG2	THR B	164	42.480	42.967	-5.234	1.00 57.23	В
		C	THR B		42.012	44.318	-1.642	1.00 57.80	В
ATOM	2703								
ATOM	2704	0	THR E	164	40.866	44.766	-1.555	1.00 57.08	В
ATOM	2705	N	PRO E	165	42.976	44.658	-0.770	1.00 58.98	В
	2706	CD	PRO E		44.315	44.055	-0.647	1.00 59.54	В
MOTA									В
MOTA	2707	CA	PRO E	165	42.734	45.605	0.322	1.00 60.52	
ATOM	2708	CB	PRO E	165	44.063	45.608	1.078	1.00 60.33	В
ATOM	2709	CG	PRO E	1 165	44.604	44.236	0.822	1.00 60.42	В
						47.002	-0.163	1.00 61.65	В
MOTA	2710	C	PRO E		42.347				
MOTA	2711	0	PRO E	165	43.149	47.698	-0.790	1.00 61.24	В
MOTA	2712	N	GLN E	3 166	41.110	47.395	0.126	1.00 62.45	В
	2713	CA	GLN F		40.598	48.709	-0.250	1.00 63.32	В
MOTA								1.00 65.46	
MOTA	2714	CB	GTN E		39.605	48.590	-1.410		В
MOTA	2715	CG	GLN F	3 166	40.177	47.945	-2.661	1.00 69.00	В
ATOM	2716	CD	GLN F	3 166	39.195	47.942	-3.819	1.00 71.19	В
							-3.697	1.00 72.48	В
MOTA	2717		GLN E		38.071	47.448			
MOTA	2718	NE2	GLN I	3 166	39.617	48.492	-4.954	1.00 72.65	В
ATOM	2719	C	GLN I	3 166	39.893	49.287	0.970	1.00 62.65	В
						48.635	1.550	1.00 62.16	В
MOTA	2720	0	GLN I		39.021				-
ATOM	2721	N	ARG I	3 167	40.266	50.501	1.366	1.00 61.62	В
MOTA	2722	CA	ARG I	3 167	39.645	51.111	2.535	1.00 60.86	В
			-	B 167	40.190	52.525	2.777	1.00 62.57	В
ATOM	2723	CB							
ATOM	2724	CG	ARG 1	B 167	39.953	53.029	4.204	1.00 64.82	В
ATOM	2725	CD	ARG I	B 167	40.742	52.198	5.227	1.00 67.31	В
				B 167	40.094	52.143	6.539	1.00 69.03	В
MOTA	2726	NE							
MOTA	2727	$^{\rm cz}$		B 167	40.570		7.591	1.00 69.14	В
ATOM	2728	NHI	ARG 1	B 167	41.710	50.804	7.499	1.00 69.34	В
			ARG		39.897		8.735	1.00 69.52	В
MOTA	2729							1.00 59.19	В
MOTA	2730	С		B 167	38.136		2.333		
MOTA	2731	0	ARG :	B 167	37.647	51.615	1.303	1.00 58.60	В
									70
P-M-JM	2722	N	GT.V	B 168	37.404	50.656	3.320	1.00 58.18	В
MOTA MOTA	2732 2733	n Ca	GLY :	B 168 B 168	37.404 35.959		3.320 3.226	1.00 58.18	В

3.004	0024	~	CTV D 160	35.466	49.200	3.191	1.00 55.42	В
MOTA	2734	C	GLY B 168					
ATOM	2735	0	GLY B 168	34.306	48.924	3.495	1.00 55.98	В
ATOM	2736	N	ASP B 169	36.350	48.280	2.814	1.00 53.44	В
ATOM	2737	CA	ASP B 169	35.979	46.871	2.757	1.00 51.76	В
ATOM	2738	CB	ASP B 169	36.841	46.115	1.740	1.00 50.49	В
						0.311	1.00 50.57	В
ATOM	2739	CG	ASP B 169	36.428	46.392			
ATOM	2740	OD1	ASP B 169	35.207	46.479	0.060	1.00 49.92	В
ATOM	2741	OD2	ASP B 169	37.318	46.507	-0.559	1.00 49.84	В
ATOM	2742	C	ASP B 169	36.083	46.181	4.110	1.00 49.36	В
						4.836	1.00 48.92	В
ATOM	2743	0	ASP B 169	37.066	46.343			
MOTA	2744	N	VAL B 170	35.047	45.418	4.436	1.00 47.48	В
ATOM	2745	CA	VAL B 170	34.981	44.667	5.680	1.00 45.10	В
ATOM	2746	CB	VAL B 170	33.800	45.130	6.543	1.00 45.86	В
						7.795	1.00 46.26	В
ATOM	2747		VAL B 170	33.702	44.268			
MOTA	2748	CG2	VAL B 170	33.974	46.598	6.906	1.00 46.23	В
ATOM	2749	С	VAL B 170	34.787	43.191	5.342	1.00 43.62	В
ATOM	2750	0	VAL B 170	33.774	42.807	4.762	1.00 42.86	В
				35.762	42.367	5.704	1.00 41.69	В
MOTA	2751	N	TYR B 171					
ATOM	2752	CA	TYR B 171	35.694	40.935	5.425	1.00 38.95	В
ATOM	2753	CB	TYR B 171	37.044	40.455	4.899	1.00 37.52	В
ATOM	2754	CG	TYR B 171	37.405	41.031	3.553	1.00 38.12	В
					40.391	2.376	1.00 37.52	В
ATOM	2755		TYR B 171	37.023				
ATOM	2756	CEI	TYR B 171	37.342	40.923	1.131	1.00 38.06	В
ATOM	2757	CD2	TYR B 171	38.118	42,224	3.454	1.00 37.54	В
ATOM	2758	CE2		38.442	42.767	2.216	1.00 38.45	В
			TYR B 171		42.110	1.056	1.00 39.25	В
ATOM	2759	CZ		38.052				
ATOM	2760	ОН	TYR B 171	38.372	42.641	-0.172	1.00 38.84	В
MOTA	2761	C	TYR B 171	35.314	40.139	6.671	1.00 37.46	В
MOTA	2762	0	TYR B 171	35.791	40.428	7.773	1.00 34.85	В
				34.452	39.140	6.501	1.00 35.06	В
MOTA	2763	N	THR B 172					В
ATOM	2764	CA	THR B 172	34.049	38.328	7.638	1.00 35.81	
ATOM	2765	CB	THR B 172	32.589	38.622	8.064	1.00 38.37	В
ATOM	2766	OG1	THR B 172	31.688	38.177	7.043	1.00 42.02	В
	2767	CG2		32.390	40.119	8.292	1.00 39.83	В
ATOM							1.00 33.71	В
MOTA	2768	C	THR B 172	34.182	36.830	7.406		
ATOM	2769	0	THR B 172	33.953	36.335	6.300	1.00 32.99	В
ATOM	2770	N	CYS B 173	34.578	36.123	8.463	1.00 32.09	В
ATOM	2771	CA	CYS B 173	34.714	34.670	8.438	1.00 31.08	В
				33.497	34.183	9.200	1.00 30.92	В
MOTA	2772	C	CYS B 173					
MOTA	2773	0	CYS B 173	33.240	34.614	10.326	1.00 32.70	В
MOTA	2774	CB	CYS B 173	35.988	34.214	9.155	1.00 31.48	В
ATOM	2775	SG	CYS B 173	36.338	32.436	8.983	1.00 31.85	В
			HIS B 174	32.748	33.288	8.578	1.00 30.26	В
ATOM	2776	N					1.00 29.72	В
MOTA	2777	CA	HIS B 174	31.524	32.754	9.152		
ATOM	2778	CB	HIS B 174	30.401	32.977	8.128	1.00 30.80	В
MOTA	2779	CG	HIS B 174	29.030	32.625	8.615	1.00 32.90	В
ATOM	2780		HIS B 174	28.016	33.405	9.058	1.00 33.11	В
						8.621	1.00 34.85	В
ATOM	2781		L HIS B 174		31.332			
ATOM	2782	CE1	HIS B 174	27.299	31.332	9.044	1.00 37.21	В
MOTA	2783	NE	HIS B 174	26.950	32.577	9.316	1.00 34.95	В
ATOM	2784	C	HIS B 174		31.271	9.449	1.00 28.49	В
					30.494	8.554	1.00 27.69	В
MOTA	2785	0	HIS B 174					
MOTA	2786	N	VAL B 175		30.888	10.710	1.00 27.48	В
MOTA	2787	CA	VAL B 175	31.810	29.508	11.121	1.00 25.94	В
ATOM	2788	CB	VAL B 179		29.418	12.126	1.00 25.31	В
					27.982	12.629	1.00 21.10	В
MOTA	2789		L VAL B 179					
ATOM	2790	CG:	2 VAL B 175		29.896	11.462	1.00 22.12	В
MOTA	2791	C	VAL B 179	30.606	28.821	11.748	1.00 26.58	В
ATOM	2792	0	VAL B 175	30.004	29.328	12.694	1.00 27.01	В
			GLU B 176		27.652	11.212	1.00 27.17	В
MOTA	2793	N					1.00 28.51	В
MOTA	2794	CA	GLU B 176		26.846	11.712		
MOTA	2795	CB	GLU B 176	28.166	26.573	10.588	1.00 32.35	В
ATOM	2796	CG	GLU B 176	27.454	27.827	10.082	1.00 38.87	В
	2797	CD				8.735	1.00 42.45	В
MOTA						8.618	1.00 43.07	В
MOTA	2798		1 GLU B 170					
MOTA	2799	ΟE:	2 GLU B 170	27.075	28.386	7.794	1.00 42.94	В
MOTA	2800	С	GLU B 170	29.750	25.536	12.235	1.00 27.34	В
ATOM	2801	ō	GLU B 17			11.574	1.00 26.12	В
						13.420	1.00 26.08	В
ATOM	2802	N	HIS B 17					В
MOTA	2803	CA				14.049	1.00 26.30	
ATOM	2804	CB	HIS B 17	7 31.132	24.244	14.738	1.00 24.58	В
MOTA	2805					15.422	1.00 22.32	В
			2 HIS B 17			14.977		В
MOTA	2806							В
MOTA	2807	ND	1 HIS B 17	7 31.437	22,711	16.710	1.00 21.01	•

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	WC	03/0969	84									
	ATOM	2808 CI	31 H	IS I	в:	177	:	32.097	21.613	17.030	1.00 23.72	В
•	ATOM	2809 N	32 H					32.838	21.255	15.995	1.00 23.87	В
	ATOM	2810 C		IS I				28.762 28.059	23.413 24.205	15.057 15.672	1.00 27.87 1.00 29.54	B B
	ATOM ATOM	2811 O 2812 N		RO I				28.654	22.085	15.237	1.00 29.57	В
	ATOM	2813 CI		RO I				29.365	21.025	14.501	1.00 28.96	В
	ATOM	2814 C	A P	RO 1	В	178		27.687	21.497	16.175	1.00 31.71	В
	ATOM	2815 CI		RO I				28.062	20.019 19.810	16.166 14.769	1.00 30.49 1.00 30.01	B B
	MOTA MOTA	2816 CC 2817 C		RO I				28.503 27.649	22.071	17.595	1.00 33.29	В
	ATOM	2818 0		RO				26.619	22.020	18.256	1.00 35.00	В
	ATOM	2819 N		ER :				28.762	22.615	18.067	1.00 34.96	В
	ATOM	2820 C		ER :				28.813	23.168 23.228	19.418 19.896	1.00 36.85 1.00 35.35	B B
	MOTA MOTA	2821 C		BR BR				30.261 31.023	24.053	19.034	1.00 35.14	В
	MOTA	2823 C		ER				28.206	24.564	19.522	1.00 38.40	В
	ATOM	2824 0		ER				27.953	25.056	20.619	1.00 37.27	В
	ATOM	2825 N		EU				27.971	25.192	18.377	1.00 40.10 1.00 41.36	B B
•	ATOM	2826 C		EU				27.434 28.162	26.545 27.352	18.340 17.269	1.00 39.74	В
	ATOM ATOM	2827 C		EU				29.677	27.432	17.422	1.00 39.93	В
	ATOM	2829 C	D1 I	EU	В	180		30.286	28.013	16.157	1.00 39.41	В
	ATOM	-	D2 I					30.021	28.279	18.636 18.078	1.00 39.61 1.00 43.85	B B
	ATOM	2831 C 2832 O		EU				25.944 25.449	26.633 26.125	17.072	1.00 44.25	В
	MOTA MOTA	2832 N				181		25.230	27.289	18.984	1.00 47.20	В
	ATOM			SLN	В	181		23.794	27.475	18.814	1.00 49.93	В
	MOTA					181		23.158	27.956	20.121	1.00 52.00 1.00 56.40	B B
	ATOM		-			181 181		23.873 23.263	29.134 29.538	20.758 22.084	1.00 59.03	В
	MOTA MOTA		E1 (					22.087	29.908	22.153	1.00 60.55	В
	MOTA		E2 (					24.059	29.468	23.149	1.00 58.44	В
•	MOTA	2840 C				181		23.635	28.522 28.465	17.715 16.906	1.00 49.23 1.00 49.91	B B
	MOTA	2841 C				181 182		22.712 24.560	29.474	17.688	1.00 48.48	В
	MOTA MOTA					182		24.555	30.523	16.679	1.00 47.89	В
	ATOM					182		24.241	31.879	17.314	1.00 48.68	В
	MOTA					182		25.211	32.223	18.286 16.038	1.00 50.58 1.00 45.93	B B
	ATOM	2846 C				182 182		25.938 26.945	30.550 30.354	16.714	1.00 45.13	В
	MOTA MOTA	2848 N				183		26.004	30.783	14.721	1.00 45.12	В
	ATOM					183		24.911	31.096	13.784	1.00 44.93	В
	MOTA	•				183		27.302	30.819	14.042 12.581	1.00 43.29 1.00 43.70	B B
	MOTA MOTA					183 183		26.923 25.642	31.070 31.833	12.688	1.00 44.70	В
	ATOM					183		28.254	31.876	14.593	1.00 40.67	В
	MOTA					183		27.828	32.851	15.209	1.00 40.46	В
	MOTA				_	184		29.547	31.664 32.607	14.382 14.842	1.00 37.76 1.00 35.88	B B
*	MOTA					184 184		30.550 31.759	32.607	15.468	1.00 35.00	В
.•	MOTA MOTA					184		32.907		15.657	1.00 35.57	В
	ATOM	2859	CG1	ILE	В	184		31.362	31.270	16.806	1.00 36.74	В
	MOTA					184		32.475	30.477 33.453	17.458 13.680	1.00 36.59 1.00 34.88	B B
	MOTA					184		31.040 31.412	33.453		1.00 35.06	В
	MOTA MOTA					185		31.043	34.764		1.00 34.50	В
	ATOM			THR	В	185		31.500				В
	ATOM		CB			185		30.356	36.592 37.285			B
	MOTA					185 185		29.770 29.286				В
	mota Mota		CGZ			185		32.622			1.00 33.38	В
• •	MOTA		ō			185		32.559	37.050	14.494		В
•	MOTA	2870	N			186		33.652				B
•	MOTA					186		34.791 36.041				В
	MOTA MOTA		CB CG1			3 186 3 186		37.212				В
	ATOM					3 186		35.766	35.674	14.262		В
	MOTA	2875	C			3 186		35.023				B
	MOTA		O N			3 186		35.060 35.172				В
	MOTA MOTA		n Ca			3 187 3 187		35.172				В
	MOTA	2879	CB			B 187		34.484	41.937	7 11.154	1.00 40.90	В
	Mota	2880	CG	GL	J	B 187		33.008				B
	ATOM	2881	CD	GLī	J 1	B 187		32.146	42.876	11.42	L 1.00 48.81	В

MOTA	2882		GLU B		30.909	42.739	11.545	1.00 51.77	В
ATOM	2883		GLU B		32.701 36.816	43.997 41.175	11.363 10.784	1.00 49.79 1.00 39.59	B B
ATOM ATOM	2884 2885	С 0	GLU B		37.637	40.998	11.684	1.00 39.84	В
ATOM	2886	N	TRP B		37.113	41.765	9.635	1.00 39.59	В
MOTA	2887	CA	TRP B		38.430	42.302	9.360	1.00 40.86	В
MOTA	2888	CB	TRP B		39.339	41.252	8.736	1.00 38.70 1.00 37.82	B B
ATOM	2889	CG	TRP B		40.769 41.421	41.704 42.383	8.693 7.615	1.00 37.82	В
ATOM ATOM	2890 2891	CE2			42.748	42.640	8.023	1.00 36.31	В
ATOM	2892	CE3			41.013	42.799	6.340	1.00 36.14	В
MOTA	2893	CD1			41.698	41.583	9.686	1.00 37.31	В
ATOM	2894		TRP B		42.890	42.141	9.291	1.00 37.27 1.00 37.17	B
MOTA	2895	CZ2	TRP B		43.673 41.932	43.296 43.452	7.204 5.522	1.00 37.17	В
ATOM ATOM	2896 2897	CH2	TRP B		43.249	43.694	5.960	1.00 37.13	В
ATOM	2898	C	TRP B		38.258	43.455	8.383	1.00 42.97	В
MOTA	2899	0	TRP B		37.946	43.240	7.211	1.00 42.37	В
ATOM	2900	N	ARG B		38.442	44.678	8.864 7.999	1.00 46.69 1.00 50.32	B B
ATOM ATOM	2901 2902	CA CB	ARG B		38.303 37.731	45.842 47.040	8.776	1.00 52.18	В
ATOM	2902	CG	ARG B		38.615	47.590	9.893	1.00 56.00	В
ATOM	2904	CD	ARG B	189	38.234	47.041	11,270	1.00 59.95	В
MOTA	2905	NE	ARG E		38.639	45.650	11.479	1.00 63.62	В
ATOM	2906	CZ	ARG B		39.903 40.899	45.236 46.105	11.559 11.447	1.00 64.33 1.00 65.45	B B
ATOM ATOM	2907 2908	NH2			40.172	43.951	11.760	1.00 64.46	В
MOTA	2909	C	ARG E		39.664	46.192	7.412	1.00 50.56	В
ATOM	2910	0	ARG E	189	40.680	46.119	8.100	1.00 50.34	В
MOTA	2911	N	ALA E		39.684	46.554	6.135 5.476	1.00 52.30 1.00 54.16	B B
ATOM	2912	CA CB	ALA E		40.933 40.846	46.911 46.592	3.987	1.00 55.33	В
MOTA MOTA	2913 2914	C	ALA E		41.238	48.392	5.679	1.00 55.19	В
ATOM	2915	ō	ALA E		40.300	49.147	6.023	1.00 54.90	В
MOTA	2916		ALA E		42.408	48.782	5.481	1.00 56.19	В
ATOM	2917	C	LEU		32.073 33.091	1.033 1.607	33.225 33.619	1.00 35.70 1.00 35.87	C
MOTA MOTA	2918 2919	И О	LEU (		29.791	1.906	32.702	1.00 36.17	Č
ATOM	2920	CA	LEU (		30.699	1.409	33.777	1.00 34.35	C
MOTA	2921	N	GLM (		32.105	0.072	32.307	1.00 34.64	C
MOTA	2922	CA	GLN (		33.374	-0.359 -0.823	31.737 30.294	1.00 34.20 1.00 33.55	C
ATOM ATOM	2923 2924	С 0	GLN (		33.250 32.373	-1.610	29.955	1.00 33.68	č
ATOM	2925	N		2 3	34.130	-0.329	29.418	1.00 33.74	С
MOTA	2926	CD	PRO		35.226	0.632	29.639	1.00 33.81	C
ATOM	2927	CA	PRO (		34.064	-0.742	28.015	1.00 34.77	C
MOTA	2928	CB	PRO		35.027 36.070	0.222 0.449	27.329 28.393	1.00 34.33 1.00 34.78	c
MOTA MOTA	2929 2930	CG C	PRO PRO		34.508	-2.195	27.890	1.00 34.42	Ċ
ATOM	2931	ŏ	PRO		35.435	-2.626	28.579	1.00 34.76	C
MOTA	2932	N	PHE	C 4	33.837	-2.947	27.024	1.00 31.97	C
ATOM	2933	CA	PHE		34.173	-4.355	26.812 26.632	1.00 32.26 1.00 34.22	c
MOTA MOTA	2934 2935	CB CG	PHE		32.897 32.006	-5.193 -5.235	27.852	1.00 37.02	č
ATOM	2936		1 PHB		32.481	-4.835	29.103	1.00 38.53	C
MOTA	2937		2 PHE		30.701	-5.726	27.756	1.00 40.29	C
ATOM	2938		1 PHE		31.673	-4.925	30.248	1.00 40.80 1.00 41.19	C
ATOM	2939		2 PHE		29.878 30.369	-5.824 -5.421	28.891 30.142	1.00 41.19	c
MOTA MOTA	2940 2941	CZ C	PHE PHE		35.052	-4.483	25.571	1.00 29.17	C
ATOM	2942	ō	PHE		34.655	-4.072	24.482	1.00 30.93	C
ATOM	2943	N	PRO		36.257		25.715	1.00 26.63	C
MOTA	2944	CD			36.936		26.974 24.577		C
MOTA MOTA	2945 2946				37.168 38.527				č
ATOM	2946				38.335				C
MOTA	2948		PRO	C 5	37.043	-6.569			C
MOTA	2949		PRO		36.403				C C
MOTA	2950		GLN		37.666 37.659				c
ATOM ATOM	2951 2952								C
MOTA	2953				36.170	-7.105	20.063		c
ATOM	2954		GLW	C 6					C
MOTA	2955	OE	31 GLN	C 6	36.483	-7.760	17.773	1.00 23.94	С

ATOM	2956	NE2	GLN	C	6	35.525	-5.766	18.149	1.00 20.70	С
MOTA	2957	С	GLN	C	6	38.996	-8.637	22.204	1.00 20.71	C
ATOM	2958	0	GLN	C	6	40.046	-8.008	22.105	1.00 19.85	C
ATOM	2959	N	PRO		7	38.974	-9.932	22.548	1.00 21.37	С
					7		-10.710	23.017	1.00 21.21	Č
ATOM	2960	CD .	PRO							
MOTA	2961	CA	PRO		7		-10.673	22.790	1.00 21.62	C
ATOM	2962	CB	PRO	С	7	39.783	-11.730	23.795	1.00 21.96	С
MOTA	2963	CG	PRO	С	7	38.416	-12.085	23.297	1.00 20.65	С
ATOM	2964	C	PRO		7	40.741	-11.316	21.511	1.00 24.05	C
					7		-11.577	20.588	1.00 22.84	c
ATOM	2965	0	PRO							
MOTA	2966	N	GLU		8		-11.550	21.448	1.00 26.22	C
ATOM	2967	CA	GLU	С	8	42.631	-12.215	20.292	1.00 27.00	С
ATOM	2968	CB	GLU	C	8	44.038	-11.687	19.988	1.00 27.94	C
ATOM	2969	CG	GLU	C	8	44.803	-12.494	18.915	1.00 28.38	C
ATOM	2970	CD	GLU		8		-12.649	17.589	1.00 31.32	C
								17.564	1.00 31.69	č
MOTA	2971		GTA		8		-13.309			
MOTA	2972	OE2	GLU	С	8		-12.112	16.563	1.00 29.86	C
ATOM	2973	C	GLU	C	8	42.678	-13.691	20. <del>6</del> 76	1.00 28.48	C
ATOM	2974	0	GLU	С	8	42.937	-14.029	21.829	1.00 28.74	С
ATOM	2975	N	LEU		9	42.407	-14.571	19.721	1.00 30.08	С
					9		-15.998	20.002	1.00 31.21	C
ATOM	2976	CA	LEU							Č
ATOM	2977	CB	LEU		9		-16.688	19.183	1.00 32.12	
MOTA	2978	CG	LEU	С	9	39.918	-16.072	19.302	1.00 33.78	C
ATOM	2979	CD1	LEU	C	9	38.941	-16.866	18.457	1.00 35.00	С
ATOM	2980	CD2			9	39,481	-16.061	20.761	1.00 35.59	C
	2981	Ç	LEU		9		-16.641	19.712	1.00 31.83	C
MOTA								18.658	1.00 30.94	Č
ATOM	2982	0	LEU		9		-16.415			
ATOM	2983	N	PRO	С	10		-17.442	20.657	1.00 33.31	C
ATOM	2984	CD	PRO	C	10	43.774	-17.661	22.032	1.00 33.12	C
ATOM	2985	CA	PRO	C	10	45.545	-18.097	20.439	1.00 36.08	C
ATOM	2986	CB	PRO		10	45.926	-18.590	21.836	1.00 36.62	С
		CG	PRO		10		-18.846	22.476	1.00 35.26	C
ATOM	2987								1.00 37.51	č
MOTA	2988	С	PRO		10		-19.229	19.430		
MOTA	2989	0	PRO	С	10	44.495	-20.030	19.491	1.00 39.49	C
MOTA	2990	N	TYR	C	11	46.365	-19.269	18.488	1.00 38.68	С
ATOM	2991	CA	TYR	C	11	46.392	-20.305	17.463	1.00 40.24	C
ATOM	2992	C	TYR		11		-20.782	17.290	1.00 42.03	C
							-21.967	17.586	1.00 42.72	C
MOTA	2993	0	TYR		11					c
ATOM	2994	OXI	TYR	C	11		-19.949	16.870	1.00 42.75	
ATOM	2995	CB	VAL	D	2	76.722	40.050	4.030	1.00 35.81	D
MOTA	2996	CG1	VAL	D	2	77.537	40.465	2.823	1.00 36.64	D
ATOM	2997		VAL		2	76.313	38.577	3.893	1.00 37.71	ם
		c	VAL		2	76.622			1.00 31.61	D
ATOM	2998							6.653	1.00 31.96	D
ATOM	2999	0	VAL		2	75.696				
MOTA	3000	N	VAL	D	2	78.625		5.418	1.00 32.12	D
ATOM	3001	CA	VAL	D	2	77.560	40.255	5.317	1.00 33.74	D
MOTA	3002	N	ALA	Q.	3	76.864	41.246	7.441	1.00 29.52	D
ATOM	3003	CA	ALA		3	76.053		8.653	1.00 27.92	D
					3	76.480		9.684	1.00 27.11	D
ATOM	3004	CB	ALA							D
MOTA	3005	C	ALA		3	76.128		9.286	1.00 25.71	
ATOM	3006	0	ALA	D	3	77.050	43.540	9.016	1.00 23.11	D
ATOM	3007	N	ASF	םי	4	75.152	43.070	10.137	1.00 24.26	D
MOTA	3008	CA	ASE	D (	4	75.109	44.354	10.825	1.00 24.77	D
ATOM	3009	CB	ASE		4	73.774		11.555	1.00 25.88	D
						72.595		10.611	1.00 26.24	D
MOTA	3010	CG	ASI		4				1.00 24.74	D
ATOM	3011		LASE		4	71.449		11.080		
ATOM	3012	OD2	2 ASE	P	4	72.81		9.416	1.00 28.25	D
MOTA	3013	C	ASI	<b>Q</b> 9	4	76.230	44.407	11.857	1.00 25.96	D
ATOM	3014	0	ASI	<b>D</b>	4	76.882	2 45.437	12.027	1.00 26.40	D
ATOM	3015	N	HIS		5	76.440		12.549	1.00 24.52	D
		CA	HIS		5	77.469		13.582	1.00 24.25	Đ
ATOM	3016							14.972	1.00 23.42	D
MOTA	3017	CB	HIS		5	76.83				
MOTA	3018	CG	HIS	3 D	5	76.13		15.231	1.00 26.12	D
ATOM	3019	CD:	2 HIS	σε	5	76.56	7 45.879	15.126	1.00 26.16	D
MOTA	3020		1 HIS		5	74.83	44.667	15.657	1.00 25.67	D
ATOM	3021		1 HIS		5	74.48		15.799	1.00 26.53	D
						75.51		15.484	1.00 25.96	D
MOTA	3022		2 HI		5				1.00 22.88	D
MOTA	3023			S D	5	78.24		13.492		
MOTA	3024	0	HI	S D	5	77.65		13.258	1.00 22.31	D
ATOM	3025	N	VA	L D	6	79.55		13.691	1.00 20.27	D
MOTA	3026			L D	6	80.42	1 40.815	13.657	1.00 19.49	Œ
ATOM	3027			ьĎ	6	81.41		12.486	1.00 20.45	D
ATOM	3028		1 VA		6	82.35		12.564	1.00 19.85	D
								11.161	1.00 25.29	D
MOTA	3029	CG	2 VA	עי	6	80.67	Z ZV.007	*****	2.44 20.27	_

ATOM	3030	C	VAL	D	6	81.223	40.792	14.944	1.00 18.77	D
MOTA	3031	0	VAL		6	81.767	41.812	15.352	1.00 17.70	D
MOTA	3032	И	ALA		7	81.304	39.626 39.489	15.575 16.821	1.00 18.23 1.00 18.01	ם מ
MOTA MOTA	3033 3034	CA CB	ALA ALA		7 7	82.046 81.080	39.452	18.006	1.00 17.61	Ď
ATOM	3035	c	ALA		7	82.899	38.239	16.838	1.00 17.37	ם
ATOM	3036	ō	ALA		7	82.568	37.242	16.208	1.00 19.56	D
ATOM	3037	N	SER	D	8	84.008	38.306	17.562	1.00 17.07	D
ATOM	3038	CA	Ser	D	8	. 84.892	37.158	17.712	1.00 15.46	D
MOTA	3039	CB	SER		8	86.297	37.455	17.202	1.00 12.56	D
ATOM	3040	OG	SER		8	86.324 84.932	37.492 36.904	15.789 19.201	1.00 18.97 1.00 16.39	D D
ATOM ATOM	3041 3042	C 0	SER SER		8 8	85.613	37.614	19.951	1.00 15.61	D
ATOM	3043	N	TYR		9	84.144	35.930	19.637	1.00 17.58	D
ATOM	3044	CA	TYR		9	84.096	35.587	21.044	1.00 18.51	D
ATOM	3045	CB	TYR	D	9	82.698	35.133	21.444	1.00 17.92	D
ATOM	3046	CG	TYR		9	81.730	36.290	21.362	1.00 17.41	Ð
ATOM	3047		TYR		9	82.056	37.523	21.928 21.840	1.00 16.27 1.00 15.18	D D
ATOM	3048	CE1	TYR TYR		9	81.208 80.515	38.603 36.169	20.701	1.00 17.05	D
ATOM ATOM	3049 3050	CE2	TYR		9	79.649	37.252	20.608	1.00 18.01	D
ATOM	3051	CZ	TYR		9	80.005	38.466	21.181	1.00 16.67	D
ATOM	3052	OH	TYR	D	9	79.157	39.543	21.104	1.00 20.30	D
ATOM	3053	C	TYR		9	85.120	34.508	21.115	1.00 19.92	D
ATOM	3054	0	TYR		9	84.856	33.323	21.337	1.00 17.21 1.00 22.61	D D
MOTA MOTA	3055	N CA	GLY		10 10	86.321 87.478	34.989 34.160	20.843	1.00 20.96	D
ATOM	3056 3057	C	GLY		10	88.358	34.354	19.624	1.00 18.79	D
ATOM	3058	ō	GLY		10	88.170	33.693	18.618	1.00 16.79	D
ATOM	3059	N	VAL	D	11	89.275	35.307	19.683	1.00 17.75	D
MOTA	3060	CA	VAL		11	90.256	35.394	18.616	1.00 16.92	D
MOTA	3061	CB	VAL		11	90.666	36.829 36.778	18.242 17.313	1.00 17.76 1.00 15.46	D D
MOTA	3062 3063		VAL VAL		11 11	91.873 89.522	37.544	17.544	1.00 13.00	D
ATOM ATOM	3064	C	VAL		11	91.391	34.728	19.395	1.00 17.46	D
ATOM	3065	ō	VAL		11	91.865	35.266	20.405	1.00 18.93	D
MOTA	3066	N	ASN	D	12	91.773	33.531	18.973	1.00 17.46	D
MOTA	3067	CA	asn		12	92.831	32.779	19.644	1.00 18.01	D
MOTA	3068	CB	ASN		12	92.339	31.360	19.969 20.955	1.00 16.68 1.00 16.27	D D
ATOM	3069	CG	ASN ASN		12 12	91.179 91.346	31.356 30.989	20.955	1.00 14.97	D
MOTA MOTA	3070 3071		ASN		12	90.000	31.779	20.497	1.00 14.97	ם
ATOM	3072	C	ASN		12	94.061	32.699	18.759	1.00 18.74	D
ATOM	3073	0	asn	D	12	93.963	32.373	17.578	1.00 19.66	D
MOTA	3074	N	LEU		13	95.221	32.969	19.344	1.00 20.75	D D
MOTA	3075	CA	LEU		13	96.471 96.841	32.949 34.387	18.600 18.234	1.00 22.59 1.00 24.32	D
MOTA MOTA	3076 3077	CB CG	PEO		13 13	98.215	34.672	17.632	1.00 25.29	D
ATOM	3078		LEU		13	98.355	33.966	16.289	1.00 24.58	D
ATOM	3079		LEU		13	98.380	36.177	17.475	1.00 23.52	D
MOTA	3080	C	LEU		13	97.646	32.290	19.330	1.00 22.44	D
MOTA	3081	0	LEU		13	97.900	32.578	20.494	1.00 24.67 1.00 23.69	ם
MOTA	3082	N	TYR		14 14	98.350 99.535	31.397 30.740	18.641 19.196	1.00 25.57	Ď
MOTA MOTA	3083 3084	CA CB	TYR		14	99.223	29.360	19.765	1.00 26.53	D
MOTA	3085	CG	TYR		14	100.445		20.383	1.00 28.87	D
MOTA	3086	CD	LTYR	D	14	100.872		21.668	1.00 28.57	D
MOTA	3087		TYR		14	102.032		22.218	1.00 27.29	D D
ATOM	3088		YYR YYR		14	101.209 102.369		19.664 20.204	1.00 29.65 1.00 26.94	D
MOTA MOTA	3089 3090	CE	TYP		14 14	102.773		21.477	1.00 27.22	D
ATOM	3091	OH	TYF		14	103.914		22.008	1.00 29.69	D
ATOM	3092	C	TYF		14	100.553		18.074	1.00 26.73	D
MOTA	3093	0	TYF		14	100.210		16.980	1.00 27.22	D
ATOM	3094	N	GL7		15	101.800 102.847		18.338 17.332	1.00 26.92 1.00 27.70	D D
MOTA MOTA	3095	CA	GFJ GFJ		15 15	102.847		16.710	1.00 27.70	D
ATOM	3096 3097	CB CG		1 D	15	103.534		17.704	1.00 27.78	D
MOTA	3098			1 D	15	103.806		17.044	1.00 27.70	D
MOTA	3099		1 GLI		15	103.723		17.685	1.00 31.07	D
MOTA	3100				15	104.142		15.763		D D
ATOM	3101			1 D	15	104.097 104.368		17.952 19.141		D
MOTA MOTA	3102			D R D	15 16	104.360		17.143		D
WIGHT	3103	74	021		70	271.00				

					106 070	20 024	17.611	1.00 28.04	D
MOTA	3104	CA	SER D	16	106.070 106.613	28.834	16.534	1.00 25.04	D
MOTA	3105	СВ	SER D	16		27.887		1.00 26.28	D
MOTA	3106	OG	SER D	16	106.879	28.581	15.330		D
MOTA	3107	C	SER D	16	107.155	29.824	18.024	1.00 27.77	ם
MOTA	3108	0	SER D	16	107.922	29.558	18.946	1.00 26.81	
MOTA	3109	N	TYR D	17	107.221	30.965	17.351	1.00 29.70	D
MOTA	3110	CA	TYR D	17	108.228	31.953	17.694	1.00 32.41	D
MOTA	3111	CB	TYR D	17	108.248	33.086	16.672	1.00 35.15	D
ATOM	3112	CG	TYR D	17	109.440	33.986	16.864	1.00 40.80	D
ATOM	3113		TYR D	17	110.719	33.556	16.508	1.00 43.28	D
ATOM	3114		TYR D	17	111.836	34.345	16.743	1.00 44.62	D
ATOM	3115		TYR D	17	109.308	35.235	17.460	1.00 40.97	D
		CE2	TYR D	17	110.419	36.032	17.702	1.00 44.83	D
ATOM	3116				111.679	35.580	17.341	1.00 45.74	D
ATOM	3117	CZ	TYR D	17		36.353	17.590	1.00 49.39	D
ATOM	3118	OH	TYR D	17	112.788		19.084	1.00 33.13	D
MOTA	3119	C	TYR D	17	107.954	32.525		1.00 33.23	Ď
ATOM	3120	0	TYR D	17	106.888	33.092	19.332		D
ATOM	3121	N	GTA D	18	108.930	32.383	19.981	1.00 32.74	
ATOM	3122	CA	GLY D	18	108.780	32.867	21.341	1.00 31.76	D
ATOM	3123	C	GLY D	18	108.958	31.716	22.311	1.00 32.63	D
ATOM	3124	0	GLY D	18	110.005	31.600	22.948	1.00 34.20	D
ATOM	3125	N	PRO D	19	107.946	30.840	22.452	1.00 33.13	α
ATOM	3126	CD	PRO D	19	108.029	29.606	23.256	1.00 31.73	D
ATOM	3127	CA	PRO D	19	106.663	30.906	21.741	1.00 32.71	D
ATOM	3128	СВ	PRO D	19	106.115	29.492	21.903	1.00 33.20	D
		CG	PRO D	19	106.591	29.128	23.280	1.00 31.76	D
MOTA	3129		PRO D	19	105.768	31.948	22.406	1.00 32.52	D
MOTA	3130	C			105.970	32.282	23.568	1.00 33.11	D
ATOM	3131	0	PRO D	19	104.786	32.463	21.676	1.00 31.92	D
ATOM	3132	N	SER D	20			22,246	1.00 30.99	D
MOTA	3133	CA	SER D	20	103.886	33.455		1.00 30.92	D
ATOM	3134	CB	SER D	20	104.287	34.867	21.795	1.00 33.16	D
ATOM	3135	OG	SER D	20	104.263	34.988	20.381		D
ATOM	3136	C	SER D	20	102.441	33.172	21.852	1.00 30.01	
MOTA	3137	0	SER D	20	102.179	32.428	20.902	1.00 29.42	D
ATOM	3138	N	GLY D	21	101.512	33.763	22.598	1.00 27.60	D
ATOM	3139	ÇA	GLY D	21	100.101	33.580	22.318	1.00 25.70	ď
MOTA	3140	С	GLY D	21	99.309	34.836	22.632	1.00 24.66	Ð
ATOM	3141	0	GLY D	21	99.848	35.798	23.187	1.00 23.84	D
MOTA	3142	N	GLN D	22	98.030	34.834	22.268	1.00 22.55	D
ATOM	3143	CA	GLN D		97.149	35.974	22.527	1.00 20.16	D
MOTA	3144	СВ	GLN D		97.301	37.049	21.445	1.00 18.28	D
		CG	GLN D		96.416	38.284	21.672	1.00 18.60	D
MOTA	3145	CD	GLN D		96.513	39.327	20.562	1.00 18.36	D
ATOM	3146				97.379	40.207	20.587	1.00 19.82	D
MOTA	3147		L GLN D		95.617	39.232	19.582	1.00 17.69	D
MOTA	3148		2 GLN D		95.699	35.517	22.561	1.00 18.61	D
ATOM	3149	C	GLN D					1.00 17.26	D
MOTA	3150	0	GLN D		95.301	34.638	21.790	1.00 16.42	D
ATOM	3151	N	TYR D		94.926	36.097	23.475		D
ATOM	3152	CA	TYR D	23	93.507	35.785	23.592	1.00 16.21	
ATOM	3153	CB	TYR I	23	93.212	34.839	24.762	1.00 14.97	D
MOTA	3154	CG	TYR I	23	91.750	34.438	24.798	1.00 14.24	D
MOTA	3155	CD	1 TYR I	23	91.309	33.318	24.109	1.00 14.49	D
ATOM	3156	CE	1 TYR I	23	89.969	33.004	24.029	1.00 14.23	D
MOTA	3157	CD	2 TYR I	23	90.795	35.240	25.421	1.00 13.21	Ď
ATOM	3158		2 TYR I	23	89.443	34.934	25.344	1.00 13.0B	D
ATOM	3159				89.039	33.814	24.647	1.00 12.88	D
ATOM	3160				87.710	33.471	24.566	1.00 16.44	a
ATOM	3161		TYR I		92.751	37.089	23.806	1.00 15.56	D
ATOM	3162		TYR I		93.014			1.00 16.57	D
ATOM	3163		THR I		91.811				D
					91.026				D
ATOM	3164				91.606				D
ATOM	3165				91.682				D
MOTA	3166		1 THR						D
ATOM	3167		2 THR		92.992				Ď
MOTA	3168		THR		89.604				D
MOTA	3169		THR 1		89.306				Ď
MOTA	3170	) N	HIS :		88.726				D
MOTA	3171	. CZ	HIS:		87.360				D
MOTA	3172	CE	HIS	D 25	86.326				
ATOM	3173				86.053				D
ATOM	3174		2 HIS		86.81				D
ATOM	317		1 HIS		84.87				D
ATOM	3176		31 HIS		84.92	36.064	24.689		D
ATOM	317		E2 HIS		86.08	35.59	1 24.289	1.00 13.67	D

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ATOM	3178	C	HIS		25	87.158	40.495	21.436	1.00 13.30	D
ATOM	3179	0	HIS		25	87.573	41.563	21.859	1.00 13.77	D
MOTA	3180	N	GLU	D	26	86.544	40.376	20.271	1.00 15.40	D
ATOM	3181	CA	GLU	D	26	86.318	41.540	19.434	1.00 16.53	D
ATOM	3182	CB	GLU	D	26	87.109	41.396	18.133	1.00 14.47	D
ATOM	3183	CG	GLU	D	26	88.627	41.460	18.277	1.00 14.81	D
ATOM	3184	CD	GLU		26	89.341	41.205	16.947	1.00 19.22	D
			GLU		26	88.726	41.429	15.884	1.00 22.84	D
ATOM	3185									
ATOM	3186		GLU		26	90.512	40.792	16.953	1.00 17.41	D
MOTA	3187	C	GLU	D	26	84.841	41.721	19.111	1.00 17.28	D
ATOM	3188	0	GLU	D	26	84.073	40.760	19.100	1.00 16.62	D
MOTA	3189	N	PHE	D	27	84.455	42.971	18.879	1.00 19.63	D
ATOM	3190	CA	PHE	D	27	83.092	43.313	18.494	1.00 19.71	D
ATOM	3191	CB	PHE		27	82.231	43.722	19.684	1.00 21.05	D
		CG	PHE		27	80.758	43.816	19.348	1.00 24.29	D
ATOM	3192								1.00 23.22	D
ATOM	3193		PHE		27	79.971	42.668	19.278		
ATOM	3194		PHE		27	80.169	45.047	19.073	1.00 22.47	D
ATOM	3195	CE1	PHE	D	27	78.617	42.744	18.940	1.00 24.89	D
ATOM	3196	CB2	PHE	D	27	78.818	45.132	18.733	1.00 24.72	D
MOTA	3197	CZ	PHE	D	27	78.041	43.980	18.667	1.00 22.80	D
ATOM	3198	С	PHE	D	27	83.182	44.482	17.532	1.00 18.41	D
ATOM	3199	Ō	PHE		27	83.700	45.545	17.879	1.00 19.21	D
ATOM	3200	N	ASP		28	82,680	44.272	16.321	1.00 18.46	D
								15.272		D
ATOM	3201	CA	ASP		28	82.700	45.284		1.00 18.63	
MOTA	3202	CB	ASP		28	81.702	46.404	15.568	1.00 19.29	Ð
MOTA	3203	CG	ASP	D	28	80.268	45.981	15.305	1.00 22.52	Þ
ATOM	3204	OD1	ASP	D	28	80.076	44.885	14.738	1.00 23.13	D
MOTA	3205	OD2	ASP	D	28	79.333	46.736	15.651	1.00 24.61	D
ATOM	3206	С	ASP		28	84.075	45.865	15.037	1.00 17.83	D
ATOM	3207	ō	ASP		28	84.225	47.069	14.860	1.00 20.60	D
ATOM		N	GLY		29	85.079	44.997	15.042	1.00 18.44	D
	3208								1.00 19.49	ā
MOTA	3209	CA	GLY		29	86.439	45.431	14.788		
MOTA	3210	C	GLY		29	87.218	46.011	15.949	1.00 18.93	D
ATOM	3211	0	GLY	D	29	88.382	46.359	15.784	1.00 19.51	D
MOTA	3212	N	ASP	D	30	86.595	46.122	17.117	1.00 17.91	D
MOTA	3213	CA	ASP	D	30	87.279	46.667	18.288	1.00 17.21	a
MOTA	3214	CB	ASP		30	86.499	47.858	18.831	1.00 15.85	D
MOTA	3215	CG	ASP		30	86.594	49.060	17.924	1.00 18.96	D
			ASP		30	87.731	49.515	17.668	1.00 18.56	D
MOTA	3216									D
ATOM	3217		ASP		30	85.541	49.544	17.466	1.00 19.00	
MOTA	3218	C	ASP	D	30	87.491	45.629	19.389	1.00 17.20	D
ATOM	3219	0	ASP	D	30	86.651	44.763	19.621	1.00 15.68	D
MOTA	3220	N	GLU	D	31	88.629	45.739	20.062	1.00 18.79	D
ATOM	3221	CA	GLU	D	31	89.015	44.829	21.131	1.00 17.52	D
ATOM	3222	CB	GLU		31	90.531	44.947	21.363	1.00 19.03	D
ATOM	3223	CG	GLU		31	91.074	44.215	22.579	1.00 22.08	D
						92.596	44.254	22.653	1.00 25.29	D
MOTA	3224	CD CD	GLU		31					
MOTA	3225		GLU		31	93.198	45.159	22.041	1.00 26.54	D
MOTA	3226	OE2	GLU	D	31	93.193	43.387	23.331	1.00 25.19	D
ATOM	3227	C	GLU	D	31	88.248	45.109	22.421	1.00 17.80	D
ATOM	3228	0	GLU	D	31	88.360	46.195	23.004	1.00 16.81	D
ATOM	3229	N	GLN	D	32	87.478	44.118	22.862	1.00 15.25	Ø
ATOM	3230	CA	GLN	D	32	86.685	44.230	24.085	1.00 15.53	D
ATOM	3231	СВ	GLN		32	85.502	43.260	24.044	1.00 12.86	D
ATOM					32	84.391	43.680	23.101	1.00 13.72	D
	3232	CG	GLN						1.00 16.53	D
MOTA	3233	СD	GLN		32	83.233	42.708	23.111		
MOTA	3234		GFM		32	83.407	41.526	22.838	1.00 20.27	D
ATOM	3235	NE2	GLN	D	32	82.044	43.203	23.423	1.00 17.48	D
ATOM	3236	С	GLN	D	32	87.528	43.956	25.329	1.00 16.00	D
ATOM .	3237	0	GLN	D	32	87.356	44.603	26.366	1.00 15.18	D
ATOM	3238	N	PHE		33	88.423	42.981	25.222	1.00 16.17	D
MOTA	3239	CA	PHE		33	89.315	42.638	26.321	1.00 15.74	D
						88.520		27.515	1.00 15.40	D
ATOM	3240	CB	PHE		33		42.083			D
ATOM	3241	CG	PHE		33	87.969	40.693	27.307	1.00 15.83	
MOTA	3242		PHE		33	88.781	39.572	27.480	1.00 16.23	D
MOTA	3243	CD2	PHE	D	33	86.625	40.503	26.977	1.00 17.27	D
MOTA	3244		PHE		33	88.262	38.282	27.332	1.00 15.79	a
ATOM	3245		PHB		33	86.088	39.218	26.827	1.00 15.20	D
ATOM	3246	cz	PHE		33	86.909	38.108	27.006	1.00 17.77	D
MOTA	3247	C	PHE		33	90.330	41.614	25.860	1.00 15.28	D
						90.157	40.979	24.825	1.00 15.16	D
ATOM	3248	0	PHE		33				1.00 15.54	D
MOTA	3249	N	TYR		34	91.405	41.476	26.620		
MOTA	3250	CA	TYR		34	92.414	40.480	26.314	1.00 16.00	D
MOTA	3251	CB	TYR	D	34	93.649	41.124	25.670	1.00 17.46	D

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ATOM	3252	CG	TYR		34					
MOTA	3253	CD1	TYR	D	34	95.488	41.390	27.391	1.00 21.91	D
MOTA	3254	CE1	TYR	D	34	96.295	42.174	28.221	1.00 24.17	D
ATOM	3255	CD2	TYR	D	34	94.351	43.354	26.638	1.00 20.26	D
ATOM	3256		TYR		34	95.147	44.141	27.463	1.00 24.97	D
						96.117	43.546	28.251	1.00 23.87	D
MOTA	3257	CZ	TYR		34					
MOTA	3258	OH	TYR	D	34	96.904	44.326	29.065	1.00 26.29	D
ATOM	3259	C	TYR	D	34	92.766	39.836	27.642	1.00 16.56	D
MOTA	3260	0	TYR		34	92.476	40.386	28.699	1.00 15.36	D
							38.653	27.586	1.00 18.29	D
ATOM	3261	N	VAL		35	93.354				
MOTA	3262	CA	VAL	D	35	93.768	37.971	28.795	1.00 19.11	D
ATOM	3263	CB	VAL	D	35	93.257	36.514	28.842	1.00 17.61	D
ATOM	3264	CG1	VAL	D	35	93.910	35.780	29.992	1.00 17.99	D
			VAL		35	91.744	36.493	29.003	1.00 17.82	D
ATOM	3265								1.00 19.96	D
ATOM	3266	C	VAL		35	95.290	37.950	28.813		
MOTA	3267	0	VAL	D	35	95.914	37.492	27.866	1.00 17.73	D
ATOM	3268	N	ASP	D	36	95.883	38.473	29.880	1.00 22.63	D
ATOM	3269	CA	ASP		36	97.333	38.456	30.005	1.00 24.79	D
					36	97.795	39.409	31.106	1.00 26.41	D
ATOM	3270	CB	ASP							•
ATOM	3271	CG	ASP		,36	99.298	39.574	31.131	1.00 30.12	D
ATOM	3272	OD1	ASP	D	36	100.002	38.547	31.252	1.00 32.04	D
ATOM	3273	OD2	ASP	D	36	99.776	40.726	31.028	1.00 32.20	D
ATOM	3274	c	ASP		36	97.650	37.011	30.389	1.00 25.23	D
			ASP			97.349	36.575	31.502	1.00 25.21	D
MOTA	3275	0			36					
MOTA	3276	N	LEU	D	37	98.236	36.272	29.455	1.00 23.64	D
ATOM	3277	CA	LEU	D	37	98.549	34.870	29.676	1.00 25.25	D
ATOM	3278	CB	LEU	D	37	98.992	34.232	28.355	1.00 21.08	D
ATOM	3279	CG	LEU		37	97.955	34.360	27.225	1.00 20.24	D
								25.899	1.00 17.23	D
ATOM	3280		LEU		37	98.568	33.934			
MOTA	3281	CD2	LEU	D	37	96.730	33.516	27.541	1.00 19.11	D
MOTA	3282	С	LEU	D	37	99.590	34.626	30.770	1.00 27.73	D
ATOM	3283	0	LEU	D	37	99.464	33.682	31.554	1.00 27.92	D
		N	GLY		38	100.608	35.474	30.837	1.00 29.31	D
MOTA	3284								1.00 30.44	D
MOTA	3285	CA	GLY		38	101.629	35.292	31.851		
MOTA	3286	C	GLY	D	38	101.141	35.640	33.242	1.00 32.52	D
MOTA	3287	0	GLY	D	38	101.502	34.986	34.220	1.00 34.37	D
ATOM	3288	N	ARG		39	100.309	36.669	33.335	1.00 35.10	D
	3289	CA	ARG		39	99.786	37.103	34.623	1.00 36.92	D
ATOM									1.00 39.96	σ
MOTA	3290	CB	ARG		39	99.693	38.632	34.653		
ATOM	3291	CG	ARG	D	39	101.011	39.318	34.301	1.00 44.57	D
MOTA	3292	CD	ARG	D	39	101.006	40.798	34.667	1.00 49.71	D
ATOM	3293	NE	ARG	D	39	102.240	41.484	34.270	1.00 53.08	D
		CZ	ARG		39	103.460	41.164	34.698	1.00 55.33	D
MOTA	3294								1.00 56.98	D
ATOM	3295		ARG		39	103.635	40.158	35.546		
ATOM	3296	NH2	ARG	D	39	104.512	41.859	34.282	1.00 56.80	D
MOTA	3297	С	ARG	D	39	98.429	36.476	34.924	1.00 35.86	D
ATOM	3298	0	ARG	מ	39	97.886	36.630	36.022	1.00 35.27	D
					40	97.893	35.757	33.944	1.00 34.51	D
MOTA	3299	N	LYS						1.00 33.49	D
MOTA	3300	CA	LYS		40	96.602	35.095	34.090		
ATOM	3301	CB	LYS	D	40	96.714	33.939	35.088	1.00 34.77	D
ATOM	3302	CG	LYS	D	40	95.482	33.040	35.133	1.00 41.38	D
ATOM	3303	CD	LYS	ם י	40	95.703	31.839	36.046	1.00 45.02	D
		CE	LYS		40	94.443	31.001	36.185	1.00 46.54	D
MOTA	3304						29.853	37.112	1.00 48.98	D
MOTA	3305	NZ	LYS		40	94.652				
ATOM	3306	C	LYS	D	40	95.511	36.064	34.542	1.00 30.95	D
ATOM	3307	0	LYS	D	40	94.780	35.794	35.492	1.00 28.23	ם
ATOM	3308	N	GLI	J D	41	95.401	37.197	33.858	1.00 30.54	D
	3309	CA		ם נ	41	94.384	38.175	34.210	1.00 30.41	D
ATOM						94.980	39.302	35.078	1.00 34.10	D
MOTA	3310	CB		JD	41					D
ATOM	3311	CG	GL	JD	41	96.180	40.034	34.488	1.00 41.52	
ATOM	3312	CD	GL	D	41	96.834	40.997	35.482	1.00 45.72	D
ATOM	3313	OE	L GL	ם ד	41	97.826	41.665	35.108	1.00 48.68	D
	3314		GLT		41	96.362	41.086	36.638	1.00 47.60	D
MOTA							38.766	33.014	1.00 28.03	D
MOTA	3315	C		םנ		93.651			1.00 25.49	ם
MOTA	3316	0	GL	ם ע		94.220				
ATOM	3317	N	TH	R D	42	92.364	39.006		1.00 25.48	D
ATOM	3318	CA		R D		91.488	39.582	32.224	1.00 23.42	D
ATOM	3319	CB		R D		90.035			1.00 22.07	D
						89.927			1.00 18.54	D
MOTA	3320		1 TH						1.00 20.32	ם
ATOM	3321	CG:	2 TH	R D		89.087				
ATOM	3322	C	TH	R D	42	91.615	41.098		1.00 22.29	D
ATOM	3323	0		R D		91.492	41.680	33.373	1.00 21.54	D
ATOM	3324	И		L D		91.874			1.00 21.50	D
						92.004				D
MOTA	3325	ÇA	Av	L D	. 43	J2.004	-2, 203			

ATOM	3326	CB	VAL D	43	93.428	43.584	30.697	1.00 21.56	D
ATOM	3327		VAL D	43	93.620	45.091	30.828	1.00 20.99	D
ATOM	3328	CG2	VAL D	43	94.456	42.827	31.539	1.00 19.79	D
MOTA	3329	С	VAL D	43	90.968	43.744	30.164	1.00 20.50	D
MOTA	3330	0	VAL D	43	91.045	43.513	28.959	1.00 19.49	D
ATOM	3331	N	TRP D	44	89.987	44.466	30.690	1.00 21.49	D
MOTA	3332	CA	TRP D	44	88.946	45.028	29.836	1.00 22.88	ď
MOTA	3333	CB	TRP D	44	87.685	45.326	30.649	1.00 21.57	D
ATOM	3334	CG	TRP D	44	87.167	44.129	31.372	1.00 21.99	D
MOTA	3335	CD2	TRP D	44	86.280	43.125	30.854	1.00 22.20	D
ATOM	3336	CE2	TRP D	44	86.119	42.150	31.862	1.00 22.19	D
ATOM	3337	CE3	TRP D	44	85.611	42.951	29.634	1.00 20.96	Ð
ATOM	3338	CD1	TRP D	44	87.492	43.736	32.633	1.00 23.17	D
ATOM	3339	NE1	TRP D	44	86.868	42.548	32.937	1.00 23.70	D
ATOM	3340	CZ2	TRP D	44	85.311	41.016	31.693	1.00 24.30	D
ATOM	3341	CZ3	TRP D	44	84.807	41.824	29.461	1.00 22.81	D
ATOM	3342	CH2	TRP D	44	84.666	40.870	30.487	1.00 24.05	D
ATOM	3343	С	TRP D	44	89.425	46.291	29.143	1.00 23.92	D
ATOM	3344	0	TRP D	44	90.081	47.131	29.759	1.00 24.50	D
ATOM	3345	N	CYS D	45	89.098	46.417	27.859	1.00 24.24	D
ATOM	3346	CA	CYS D	45	89.498	47.580	27.069	1.00 26.23	D
ATOM	3347	CB	CYS D	45	89.951	47.141	25.672	1.00 25.96	D
ATOM	3348	SG	CYS D	45	91.422	46.098	25.665	1.00 25.42	D
MOTA	3349	C	CYS D	45	88.377	48.608	26.950	1.00 27.07	D
ATOM	3350	0	CYS D	45	88.612	49.749	26.549	1.00 28.23	D
MOTA	3351	N	LEU D	46	87.157	48.193	27.273	1.00 27.18	D
MOTA	3352	CA	LEU D	46	86.002	49.087	27.232	1.00 28.16	D
MOTA	3353	CB	LEU D	46	84.907	48.525	26.320	1.00 27.82	D
ATOM	3354	CG	LEU D	46	84.142	49.460	25.372	1.00 30.22	D
ATOM	3355	CD1	LEU D	46	82.792	48.827	25.040	1.00 29.72	D
ATOM	3356	CD2	LEU D	46	83.928	50.827	25.994	1.00 31.10	D
ATOM	3357	C	LEU D	46	85.504	49.138	28.675	1.00 28.73	D
MOTA	3358	0	LEU D	46	85.049	48.133	29.216	1.00 28.92	D
MOTA	3359	N	PRO D	47	85.601	50.309	29.318	1.00 29.35	D
ATOM	3360	CD	PRO D	47	86.116	51.554	28.717	1.00 28.33	D
ATOM	3361	CA	PRO D	47	85.182	50.533	30.709	1.00 29.01	D
ATOM	3362	CB	PRO D	47	B5.139	52.051	30.806	1.00 29.32	D
ATOM	3363	CG	PRO D	47	86.307	52.447	29.929	1.00 30.61	D
ATOM	3364	С	PRO D	47	83.879	49.875	31.169	1.00 28.51	D
ATOM	3365	0	PRO D	47	83.867	49.151	32.163	1.00 28.22	D
ATOM	3366	N	VAL D	48	82.784	50.126	30.458	1.00 28.05	D
ATOM	3367	CA	VAL D	48	81.492	49.545	30.826	1.00 27.41	D
ATOM	3368	СВ	VAL D	48	80.406	49.918	29.810	1.00 26.31	D
ATOM	3369		VAL D	48	79.955	51.345	30.027	1.00 30.25	D
ATOM	3370	CG2	VAL D	48	80.949	49.744	28.398	1.00 26.11	D
ATOM	3371	C	VAL D	48	81.490	48.022	30.961	1.00 26.77	D
ATOM	3372	0	VAL D	48	80.622	47.462	31.627	1.00 27.43	D
MOTA	3373	N	LEU D	49	82.449	47.353	30.332	1.00 25.75	D
ATOM	3374	CA	PEA D	49	82.517	45.898	30.395	1.00 27.21	D
MOTA	3375	CB	LEU D	49	83.237	45.354	29.153	1.00 27.47	D
MOTA	3376	CG	LEU D	49	82.405	44.886	27.944	1.00 29.74	D
ATOM	3377	CD:	L LEU D	49	81.361	45.898	27.578	1.00 29.28	D
MOTA	3378	CD:	FEG D	49	83.329	44.627	26.753	1.00 29.72	D
MOTA	3379	C	TEA D		83.185	45.374	31.674	1.00 27.86	D
MOTA	3380	0	LEU D	49	83.246	44.163	31.900	1.00 25.45	D
ATOM	3381	N	ARG D		83.680	46.283	32.508	1.00 29.82	D
MOTA	3382	CA	ARG D		84.319	45.892	33.768	1.00 32.18	D
MOTA	3383	CB	ARG D		84.900	47.105	34.509	1.00 35.49	D
MOTA	3384	CG	ARG D		86.010	47.890	33.824	1.00 40.53	D
MOTA	3385	CD	ARG D		86.524	48.968	34.786	1.00 42.89	D
MOTA	3386	NE	ARG I		87.297	50.017	34.125	1.00 46.26	D
MOTA	3387				88.484	49.836	33.555	1.00 46.43	D
MOTA	3388		1 ARG D		89.049	48.636	33.564	1.00 46.42	D
MOTA	3389	NH	2 ARG I		89.100	50.857	32.968	1.00 43.78	D
MOTA	3390		ARG I		83.283	45.247	34.690	1.00 31.58	D D
MOTA	3391		ARG I		83.631	44.577	35.664	1.00 31.56	
ATOM	3392		GTN I		82.009	45.476	34.397	1.00 30.22	D
MOTA	3393				80.942	44.921	35.221	1.00 30.10	D D
ATOM	3394				79.610	45.592	34.880	1.00 31.37 1.00 33.44	D
MOTA	3395				79.194	45.469	33.426	1.00 37.07	
MOTA	3396				77.888	46.188	33.144	1.00 37.07	D D
MOTA	3397		1 GLN I		76.835		33.678		D
MOTA	3398		2 GLN I		77.951				D
MOTA	3399	C	GLN 1	D <b>51</b>	80.830	43.411	35.049	T.00 23.31	,

								- 00 00 00	_
ATOM	3400	o	GLN D	51	80.291	42.721	35.911	1.00 29.09	D
MOTA	3401	N	PHE D	52	81.342	42.899	33.935	1.00 28.19	D
ATOM	3402	CA	DHE D	52	81.300	41.468	33.676	1.00 26.27	D
ATOM	3403	СВ	PHE D	52	81.218	41.188	32.178	1.00 25.00	D
	3404	CG	PHE D	52	80.030	41.801	31.513	1.00 23.07	D
ATOM			PHE D		78.744	41.569	31.999	1.00 22.75	D
ATOM	3405			52				1.00 23.46	D
MOTA	3406	CD2	PHE D	52	80.188	42.594	30.380		
ATOM	3407	CE1	PHE D	52	77.627	42.122	31.364	1.00 21.26	D
ATOM	3408	CE2	PHE D	52	79.079	43.151	29.735	1.00 21.92	D
ATOM	3409	CZ	PHE D	52	77.799	42.913	30.231	1.00 21.69	D
ATOM	3410	C	PHE D	52	82.547	40.797	34.217	1.00 27.11	D
ATOM	3411	ō	PHE D	52	83.477	41.461	34.669	1.00 27.64	D
				53	82.556	39.471	34.152	1.00 27.25	D
ATOM	3412	N	ARG D				34.609	1.00 28.31	D
MOTA	3413	ÇA	ARG D	53	83.683	38.672			
MOTA	3414	CB	ARG D	53	83.347	37.976	35.939	1.00 32.75	D
MOTA	3415	CG	ARG D	53	83.263	38.921	37.143	1.00 40.59	D
MOTA	3416	CD	ARG D	53	82.418	38.325	38.269	1.00 45.99	D
ATOM	3417	NE	ARG D	53	81.007	38.229	37.892	1.00 52.14	D
ATOM	3418	CZ	ARG D	53	80.172	39.265	37.808	1.00 53.70	D
	3419		ARG D	53	80.597	40.493	38.080	1.00 53.85	D
ATOM					78.910	39.071	37.440	1.00 54.61	D
MOTA	3420	NH2		53					D
ATOM	3421	C	ARG D	53	84.007	37.624	33.548	1.00 25.73	
ATOM	3422	0	ARG D	53	83.120	37.103	32.875	1.00 23.84	D
ATOM	3423	N	PHE D	54	85.290	37.335	33.387	1.00 23.47	D
MOTA	3424	CA	PHE D	54	85.716	36.336	32.425	1.00 19.92	D
ATOM	3425	CB	PHE D	54	86.159	36.980	31.113	1.00 15.46	D
	3426	CG	PHE D	54	86.346	35.994	30.007	1.00 17.29	D
MOTA				54	85.249	35.506	29.303	1.00 15.32	D
MOTA	3427		PHE D					1.00 15.07	ā
ATOM	3428	CD2		54	87.615	35.503	29.701		
MOTA	3429	CE1	PHE D	54	85.415	34.539	28.309	1.00 16.04	D
ATOM	3430	CE2	PHE D	54	87.788	34.535	28.709	1.00 13.99	D
ATOM	3431	CZ	PHE D	54	86.688	34.055	28.014	1.00 14.35	D
MOTA	3432	C	PHE D	54	86.879	35.598	33.055	1.00 18.63	D
		ō	PHE D	54	87.922	36.188	33.329	1.00 19.50	D
ATOM	3433					34.312	33.309	1.00 19.05	D
MOTA	3434	N	ASP D	55	86.676				D
ATOM	3435	CA	ASP D	55	87.689	33.466	33.921	1.00 19.33	
MOTA	3436	CB	ASP D	55	87.084	32.100	34.237	1.00 21.38	D
MOTA	3437	CG	ASP D	55	88.090	31.138	34.832	1.00 24.95	D
ATOM	3438	OD1	ASP D	55	89.264	31.528	35.021	1.00 27.01	D
ATOM	3439		ASP D	55	87.703	29.985	35.112	1.00 27.48	D
		C	ASP D	55	88.863	33.323	32.955	1.00 19.84	D
MOTA	3440				88.741	32.691	31.904	1.00 18.07	α
MOTA	3441	0	ASP D	55				1.00 19.36	D
ATOM	3442	N	PRO D	56	90.024	33.909	33.311		
MOTA	3443	CD	PRO D	56	90.285	34.584	34.593	1.00 16.09	D
ATOM	3444	CA	PRO D	56	91.240	33.867	32.486	1.00 18.34	D
MOTA	3445	CB	PRO D	56	92.228	34.729	33.278	1.00 19.78	D
ATOM	3446	CG	PRO D	56	91.792	34.517	34.692	1.00 18.66	a
		c	PRO D	56	91.770	32.468	32.206	1.00 18.30	D
MOTA	3447					32.277	31.299	1.00 17.41	D
MOTA	3448	0	PRO D	56	92.583			1.00 18.31	ם
MOTA	3449	N	GLW D	57	91.304	31.489	32.977		
MOTA	3450	CA	GLN D	57	91.744	30.114	32.781	1.00 18.39	D
MOTA	3451	CB	GLN D	57	91.314	29.233	33.963	1.00 19.94	D
ATOM	3452	CG	GLN D	57	91.738	27.773	33.856	1.00 18.50	D
ATOM	3453	CD	GLN D		93.252	27.603	33.765	1.00 23.86	D
ATOM	3454	OE:			94.000	28.110	34.612	1.00 23.68	D
					93.709	26.885	32.739	1.00 19.56	D
MOTA	3455	NE:				29.555	31.480	1.00 20.01	D
MOTA	3456	C	GTN D		91.174			1.00 19.26	D
ATOM	3457	0	GLN D		91.733	28.618	30.903		
MOTA	3458	N	PHE D	58	90.059	30.113	31.016	1.00 19.19	D
MOTA	3459	CA	PHE D	58	89.490	29.629	29.765	1.00 20.37	D
ATOM	3460		PHE D	58	88.178	30.347	29.427	1.00 18.69	D
MOTA	3461		PHE D		87.587	29.912	28.114	1.00 20.67	D
			1 PHE D		88.040	30.456	26.912	1.00 19.84	D
ATOM	3462						28.070	1.00 19.87	D
MOTA	3463		2 PHE D		86.640	28.891			D
MOTA	3464		1 PHE D		87.562	29.984	25.682	1.00 19.25	
MOTA	3465	CE	2 PHE D	58	86.156	28.411	26.844	1.00 20.67	D
MOTA	3466	CZ	PHE D	58	86.623	28.961	25.652	1.00 19.50	D
ATOM	3467		PHE D	58	90.508	29.892	28.659	1.00 20.46	D
ATOM	3468		PHE I		90.745	29.049	27.790	1.00 20.36	D
			ALA I		91.115	31.070	28.716	1.00 20.85	D
MOTA	3469				92.111	31.477	27.736	1.00 21.87	D
MOTA	3470								D
MOTA	3471				92.458	32.959	27.937		
MOTA	3472	C	ALA I		93.374	30.618	27.819		D
MOTA	3473	0	ALA I	59	93.877	30.151	26.796	1.00 22.54	D

				_	<b>CO</b>	93.890	30.409	29.030	1.00 21.24	D
MOTA	3474	N	LEU		60		29.601	29.188	1.00 22.31	D
MOTA	3475	CA	FEA		60	95.101			1.00 22.79	Ď
ATOM	3476	CB	PRA		60	95.501	29.474	30.663	1.00 25.87	D
ATOM	3477	CG	LEU		60	96.063	30.698	31.393		D
ATOM	3478	CD1			60	96.455	30.303	32.805	1.00 28.75	
MOTA	3479	CD2			60	97.270	31.223	30.670	1.00 28.42	D
MOTA	3480	С	LEU	D	60	94.891	28.207	28.617	1.00 21.85	D
MOTA	3481	0	LEU	D	60	95.731	27.691	27.875	1.00 22.48	D
ATOM	3482	N	THR	D	61	93.763	27.600	28.966	1.00 19.32	D
MOTA	3483	CA	THR	D	61	93.457	26.259	28,489	1.00 20.67	D
MOTA	3484	CB	THR	D	61	92.175	25.721	29.158	1.00 20.04	D
ATOM	3485	0G1	THR	D	61	92.419	25.539	30.558	1.00 23.09	D
ATOM	3486		THR		61	91.759	24.393	28.546	1.00 21.15	D
ATOM	3487	C	THR		61	93.283	26.240	26.974	1.00 19.50	D
ATOM	3488	ō	THR		61	93.805	25.363	26.288	1.00 18.76	D
ATOM	3489	N	ASN		62	92.565	27.229	26.456	1.00 19.66	α
ATOM	3490	CA	ASN		62	92.310	27.300	25.032	1.00 19.00	D
		CB	ASN		62	91.356	28.453	24.729	1.00 18.52	D
MOTA	3491		ASN		62	90.262	28.052	23.760	1.00 20.31	D
ATOM	3492	CG			62	89.726	26.942	23.833	1.00 19.27	D
MOTA	3493		ASN		62	89.917	28.952	22.854	1.00 22.25	D
ATOM	3494		ASN			93.599	27.445	24.244	1.00 19.63	ם
ATOM	3495	C	ASN		62		26.788	23.221	1.00 21.16	D
MOTA	3496	0	ASN		62	93.774		24.724	1.00 19.68	D
ATOM	3497	N	ILE		63	94.509	28.290		1.00 18.76	D
ATOM	3498	CA	ILE		63	95.779	28.481	24.033	1.00 18.70	D
ATOM	3499	CB	ILE		63	96.587	29.660	24.645		
MOTA	3500	CG2			63	97.946	29.780	23.966	1.00 17.99	D
ATOM	3501		ILE		63	95.813	30.968	24.471	1.00 17.09	D
ATOM	3502	CD1	ILE	D	63	95.507	31.313	23.017	1.00 17.47	D
ATOM	3503	C	ILE	D	63	96.613	27.195	24.094	1.00 18.86	D
MOTA	3504	0	ILE	D	63	97.354	26.885	23.164	1.00 20.67	D
ATOM	3505	N	ALF	D	64	96.497	26.448	25.188	1.00 18.22	D
ATOM	3506	CA	ALA	D	64	97.244	25.193	25.316	1.00 20.33	D
ATOM	3507	СВ	AL/	A D	64	97.039	24.574	26.708	1.00 17.30	D
ATOM	3508	C	AL/		64	96.756	24.232	24.233	1.00 21.38	D
ATOM	3509	ō	AL		64	97.536	23.459	23.677	1.00 23.44	D
ATOM	3510	N	VAI		65	95.459	24.290	23.940	1.00 21.97	α
ATOM	3511	CA	VAI		65	94.872	23.444	22.910	1.00 22.59	D
	3512	СВ	VAI		65	93.324	23.570	22.890	1.00 22.30	D
ATOM	3513		. VAI		65	92.744	22.781	21.728	1.00 17.73	D
ATOM		CG2			65	92.747	23.053	24.204	1.00 19.10	D
ATOM	3514				65	95.441	23.832	21.541	1.00 23.65	D
MOTA	3515	C		. D		95.783	22.961	20.746	1.00 23.24	D
ATOM	3516	0		r D	65	95.552	25.133	21.271	1.00 25.03	D
ATOM	3517	N		J D	66		25.580	19.991	1.00 26.10	D
MOTA	351B	CA		D D	66	96.102	27.111	19.870	1.00 23.98	ď
MOTA	3519	CB		O D	66	96.104		19.969	1.00 25.20	D
MOTA	3520	CG		D D	66	94.826	27.953	19.169	1.00 21.70	D
MOTA	3521		LE		66	95.030	29.233		1.00 26.16	D
ATOM	3522		FE		66	93.629	27.211	19.435	1.00 26.24	D
MOTA	3523	C		UΡ	66	97.533	25.078	19.880	1.00 28.24	D
MOTA	3524	0		υD	66	97.971	24.667	18.816		D
MOTA	3525	N		S D	67	98.262	25.131	20.989	1.00 27.93	
MOTA	3526	CA	ĽΥ	S D	67	99.642	24.658	21.024	1.00 28.00	D
MOTA	3527	CB	LY	S D	67	100.215	24.827	22.437	1.00 27.69	D
MOTA	3528	CG	LY	S D	67	101.633	24.316		1.00 28.46	D
MOTA	3529	CD	LY	S D	67	102.086	24.504		1.00 30.94	D
MOTA	3530	CE	LY	S D	67	103.401	23.791		1.00 32.95	Q
ATOM	3531	NZ	LY	S D	67	104.517	24.279	23.503	1.00 35.64	D
ATOM	3532	С	ΓĀ	s d	67	99.642	23.182	20.629		D
ATOM	3533	0		S D		100.414	22.759	19.767	1.00 27.65	D
ATOM	3534			SD		98.761	22.405	21.254	1.00 27.05	D
ATOM	3535			SE		98.665	_	20.956	1.00 26.31	D
MOTA	3536			SI		97.600			1.00 27.74	D
				SE		97.356			1.00 31.20	D
MOTA	3537		2 HI			97.801				D
MOTA	3538		2 HI			96.582				D
MOTA	3539					96.560	_			ם
MOTA	3540		1 HI			97.292				D
MOTA	3541		2 H							D
MOTA	3542			is i		98.341				Ď
MOTA	3543			s I		98.958				D
ATOM	3544			SN I		97.386	21.521			D
MOTA	3545			SN I		96.986				D
ATOM	3546			SN I		95.706				D
MOTA	3547	CG	: As	SN I	69	94.447	7 21.504	17.805	24.60	ט

ATOM	3548	ODI	ASN D	69	94.521	20.536	18.562	1.00 26.69	D
ATOM	3549		ASN D	69	93.283	21.994	17.381	1.00 21.03	D
		-	ASN D	69	98.091	21.855	16.601	1.00 24.52	Ď
MOTA	3550	C				21.223	15.570	1.00 22.82	D
MOTA	3551	0	ASN D	69	98.329		16.934	1.00 24.56	D
ATOM	3552	N	LEU D	70	98.763	22.954		1.00 26.89	D
MOTA	3553	CA	TEO D	70	99.831	23.459	16.078		ā
ATOM	3554	CB	TEA D	70	100.478	24.707	16.690	1.00 23.85	
ATOM	3555	CG	TEA D	70	101.619	25.306	15.857	1.00 22.71	D
MOTA	3556	CD1	TEQ D	70	101.082	25.776	14.519	1.00 19.18	ם
MOTA	3557	CD2	LEU D	70	102.254	26.472	16.592	1.00 23.62	D
ATOM	3558	C	LEU D	70	100.900	22.388	15.882	1.00 28.63	D
ATOM	3559	0	TEA D	70	101.413	22.210	14.780	1.00 27.56	D
ATOM	3560	N	ASN D	71	101.224	21.687	16.967	1.00 31.13	D
ATOM	3561	CA	ASN D	71	102.238	20.637	16.962	1.00 35.25	D
ATOM	3562	СВ	ASN D	71	102.393	20.052	18.370	1.00 35.30	D
ATOM	3563	CG	ASN D	71	103.149	20.978	19.307	1.00 38.03	D
ATOM	3564		ASN D	71	103.197	20.751	20.518	1.00 40.05	D
ATOM	3565		ASN D	71	103.752	22.026	18.748	1.00 38.78	D
ATOM	3566	c	ASN D	71	101.931	19.521	15.975	1.00 36.85	D
MOTA	3567	ō	ASN D	71	102.829	18.997	15.316	1.00 36.91	D
		N	SER D	72	100.660	19.157	15.876	1.00 38.08	D
ATOM	3568			72	100.261	18.104	14.961	1.00 39.44	D
ATOM	3569	CA	SER D		98.847	17.623	15.306	1.00 40.69	Ď
ATOM	3570	CB	SER D	72		16.427	14.611	1.00 44.84	D
MOTA	3571	OG	SER D	72	98.529		13.520	1.00 39.55	D
ATOM	3572	С	SER D	72	100.320	18.614		1.00 38.61	D
MOTA	3573	0	SER D	72	100.798	17.915	12.625		D
ATOM	3574	N	TRO D	73	99.846	19.839	13.305	1.00 40.64	
MOTA	3575	CA	TEO D	73	99.844	20.443	11.974	1.00 42.19	D
MOTA	3576	CB	LEU D	73	99.085	21.768	11.990	1.00 42.17	D
ATOM	3577	CG	TEO D	73	97.608	21.700	11.608	1.00 43.12	D
ATOM	3578	CD1	PEA D	73	96.891	20.664	12.443	1.00 44.19	D
ATOM	3579	CD2	PEA D	73	96.988	23.072	11.801	1.00 44.59	D
ATOM	3580	C	LEU D	73	101.237	20.678	11.407	1.00 43.27	D
MOTA	3581	0	LEU D	73	101.466	20.479	10.215	1.00 43.00	D
ATOM	3582	N	ILE D	74	102.162	21.116	12.253	1.00 44.60	ם
ATOM	3583	CA	ILE D	74	103.529	21.364	11.812	1.00 46.44	D
MOTA	3584	СВ	ILE D	74	104.431	21.770	13.000	1.00 46.31	D
MOTA	3585	CG2		74	105.893	21.792	12,571	1.00 46.14	D
	3586	CG1		74	103.996	23.140	13.529	1.00 45.97	D
MOTA			ILE D	74	104.683	23.561	14.812	1.00 43.97	D
MOTA	3587				104.003	20.095	11.166	1.00 48.14	D
MOTA	3588	C	ILE D	74	104.724	20.147	10.119	1.00 48.28	D
ATOM	3589	0	IPE D	74			11.795	1.00 49.68	D
MOTA	3590	N	LYS D	75	103.800	18.957		1.00 51.82	D
MOTA	3591	CA	LYS D	75	104.252	17.669	11.290		D
ATOM	3592	СВ	LYS D	75	104.060	16.589	12.356	1.00 52.85	
ATOM	3593	ÇG	LYS D	75	104.856	16.839	13.621	1.00 54.78	D
ATOM	3594	CD	LYS D	75	104.517	15.831	14.704	1.00 57.28	D
MOTA	3595	CE	LYS D	75	105.222	16.170	16.010	1.00 58.75	D
MOTA	3596	NZ	LYS D	75	104.803	15.266	17.116	1.00 59.97	D
ATOM	3597	C	LYS D	75	103.499	17.276	10.023	1.00 52.37	D
MOTA	3598	0	LYS D	75	104.106	17.086	8.972	1.00 52.78	D
MOTA	3599	N	ARG D	76	102.177	17.171	10.124	1.00 52.67	D
ATOM	3600	CA	ARG D	76	101.353	16.783	8.986	1.00 52.67	D
ATOM	3601	СВ	ARG D		99.911	16.546	9.439	1.00 53.54	D
ATOM	3602	CG	ARG D		99.764	15.339	10.346	1.00 55.62	Œ
ATOM	3603	CD	ARG D		98.310	15.011	10.639	1.00 58.29	D
ATOM	3604	NE	ARG D		97.628	16.107	11.319	1.00 61.07	D
MOTA	3605	CZ	ARG I		96.437	16.000	11.900	1.00 62.21	D
MOTA	3606		ARG D		95.793	14.840	11.885	1.00 62.71	D
			2 ARG I		95.889	17.055	12.492	1.00 61.94	D
ATOM	3607		ARG I		101.375	17.761	7.816	1.00 52.35	D
MOTA	3608	C			100.691	17.550	6.817	1.00 52.65	D
MOTA	3609	0	ARG I		102.160	18.824	7.932	1.00 52.02	D
MOTA	3610	N	SER I				6.856	1.00 51.87	D
MOTA	3611		SER I		102.255		7.379	1.00 50.95	D
MOTA	3612		SER I		101.945	21.212	8.239		D
MOTA	3613				102.975			1.00 48.11	ם
MOTA	3614		SER I		103.667		6.287	1.00 52.25	
ATOM	3615	0	SER I		104.028		5.464	1.00 51.67	D
MOTA	3616	N	asn i		104.455		6.731	1.00 52.79	D
MOTA	3617	CA	ASN 1	78	105.841			1.00 53.67	D
ATOM	3618	CB	ASN I	78	105.912			1.00 55.53	D
MOTA	3619		ASN I	78	107.298				D
ATOM	3620		1 ASN 1		107.959				D
ATOM	3621		2 ASN 1		107.732	18,360	3.184	1.00 58.05	D
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MOTA	3622	C	asn		78	106.549	19.985	6.632	1.00 52.90	D
MOTA	3623	0	asn	D	78	107.300	20.536	5.826	1.00 53.98	D
MOTA	3624	N	SER	D	79	106.275	20.479	7.835	1.00 51.25	D.
ATOM	3625	CA	SER	D	79	106.856	21.715	8.341	1.00 49.59	D
ATOM	3626	CB	SER		79	108.333	21.498	8.664	1.00 49.69	D
			SER		79	108.472	20.604	9.753	1.00 52.23	D
ATOM	3627	OG								Ď
MOTA	3628	С	SER		79	106.711	22.931	7.437	1.00 47.21	
MOTA	3629	0	SER	D	79	107.699	23.588	7.111	1.00 47.49	D
MOTA	3630	N	THR	D	80	105.483	23.235	7.032	1.00 44.68	D
ATOM	3631	CA	THR	D	80	105.245	24.401	6.189	1.00 43.69	D
ATOM	3632	CB	THR	D	80	103.928	24.274	5.407	1.00 45.12	D
ATOM	3633		THR		80	103.976	23.112	4.570	1.00 47.94	D
ATOM		CG2			80	103.706	25.505	4.541	1.00 44.11	D
	3634					105.166	25.634	7.094	1.00 42.94	ם
ATOM	3635	C	THR		80					
MOTA	3636	0	THR		80	104.225	25.783	7.874	1.00 41.60	D
ATOM	3637	N	ALA	D	81	106.162	26.510	6.988	1.00 40.39	D
MOTA	3638	CA	ALA	D	81	106.215	27.715	7.804	1.00 37.86	Ð
MOTA	3639	CB	ALA	D	81	107.657	28.171	7.958	1.00 39.23	D
ATOM	3640	C	ALA	D	81	105.372	28.846	7.234	1.00 36.29	D
ATOM	3641	ō	ALA		81	104.988	28.829	6.065	1.00 35.21	D
ATOM	3642	N	ALA		82	105.087	29.829	8.079	1.00 34.40	D
						104.294	30.984	7.685	1.00 32.51	D
ATOM	3643	CA	ALA		82					Ď
MOTA	3644	CB	ALA		82	103.915	31.789	8.920	1.00 32.45	
ATOM	3645	С	ALA	D	82	105.064	31.866	6.707	1.00 32.78	D
ATOM	3646	0	ALA	D	82	106.294	31.913	6.740	1.00 30.87	D
ATOM	3647	N	THR	D	83	104.333	32.561	5.839	1.00 32.79	D
ATOM	3648	CA	THR	D	83	104.940	33.459	4.867	1.00 34.48	D
MOTA	3649	CB	THR		83	104.195	33.429	3.521	1.00 35.64	g
			THR		83	104.179	32.094	3.006	1.00 38.88	D
ATOM	3650							2.521	1.00 35.33	D
MOTA	3651	CG2			83	104.880	34.342			
MOTA	3652	С	THR		83	104.886	34.887	5.401	1.00 35.30	D
MOTA	3653	0	THR	D	83	103.827	35.355	5.824	1.00 36.88	D
MOTA	3654	N	ASN	D	84	106.025	35.575	5.379	1.00 35.07	D
MOTA	3655	CA	ASN	D	84	106.095	36.949	5.855	1.00 33.90	D
ATOM	3656	СВ	ASN		84	107.548	37.413	6.010	1.00 34.23	D
ATOM	3657	CG	ASN		84	108.351	36.545	6.954	1.00 36.16	D
			ASN		84	107.895	36.195	8.043	1.00 34.99	D
ATOM	3658							6.545	1.00 37.40	D
ATOM	3659		ASN		84	109.572	36.205			D
ATOM	3660	С	asn		84	105.419	37.879	4.865	1.00 34.74	
MOTA	3661	0	asn	D	84	105.814	37.940	3.699	1.00 35.59	D
ATOM	3662	N	GTU	D	85	104.401	38.599	5.327	1.00 34.09	D
ATOM	3663	CA	GLU	D	85	103.695	39.561	4.489	1.00 32.99	D
ATOM	3664	CB	GLU	D	85	102.239	39.714	4.939	1.00 35.56	D
ATOM	3665	CG	GLU		85	101.370	38.475	4.746	1.00 40.80	D
ATOM	3666	CD	GLU		85	101.019	38.215	3.291	1.00 43.32	D
			GLU.		85	100.409	39.104	2.658	1.00 46.21	D
MOTA	3667								1.00 44.58	D
MOTA	3668		GLU		85	101.345	37.119	2.782		
ATOM	3669	C	GLU	D	85	104.418	40.886	4.681	1.00 31.21	D
MOTA	3670	0	GLD	D	85	105.220	41.024	5.602	1.00 32.36	D
MOTA	3671	N	VAL	D	86	104.140	41.848	3.808	1.00 29.71	D
ATOM	3672	CA	VAL	D	86	104.749	43.170	3.882	1.00 27.94	D
ATOM	3673	СВ	VAL		86	105.079	43.712	2.467	1.00 26.90	D
ATOM	3674		VAL		86	105.569	45.166	2.543	1.00 23.11	D
					86	106.134	42.829	1.821	1.00 24.31	D
MOTA	3675		VAL					4.574	1.00 29.81	D
MOTA	3676	C	VAL		86	103.767	44.114			
MOTA	3677	0	VAL		86	102.658	44.343	4.088	1.00 30.28	D
ATOM	3678	N	PRO	D	87	104.162	44.666	5.729	1.00 29.08	D
ATOM	3679	CD	PRO	<b>D</b>	87	105.356	44.310	6.509	1.00 29.37	Đ
MOTA	3680	CA	PRO	D	87	103.306	45.583	6.485	1.00 30.85	D
ATOM	3681	CB	PRO		87	104.083	45.791	7.786	1.00 30.80	D
ATOM	3682	CG	PRO		87	104.878	44.551	7.920	1.00 30.83	D
	3683	c	PRO		87	103.049	46.907	5.772	1.00 31.43	D
ATOM							47.357	4.968	1.00 31.78	D
MOTA	3684	0	PRO		87	103.863				
MOTA	3685	N	GLU		88	101.907	47.517	6.081	1.00 31.85	D
MOTA	3686	CA	GLU		88	101.516	48.808	5.521	1.00 32.77	Þ
MOTA	3687	CB	GLU	ם נ	88	100.195	48.687	4.744	1.00 35.18	D
ATOM	3688	CG	GLU		88	99.814	49.960	3.987	1.00 43.00	α
ATOM	3689	CD	GLU			98.512	49.839	3.205	1.00 46.30	D
ATOM	3690		1 GLU			97.439	49.745	3.837	1.00 47.40	D
	3691		2 GLU			98.564	49.840	1,954	1.00 48.25	D
MOTA							49.748	6.721	1.00 31.26	D
MOTA	3692	C	GL			101.338			1.00 31.20	D
MOTA	3693	0	GL			100.556	49.457	7.630		
MOTA	3694	N	VAI			102.060	50.864	6.728	1.00 28.43	D
MOTA	3695	CA	VAI	ם	89	101.988	51.806	7.842	1.00 26.87	D

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ATOM	3696	CB	VAL I		89	103.385	52.024	8.454		
MOTA	3697	CG1	VAL 1	D	89	103.277	52.886	9.699	1.00 26.80	ם
MOTA	3698	CG2	VAL 1	D	89	104.021	50.679	8.787	1.00 24.58	D
ATOM	3699	C	VAL I	D	89	101.389	53.174	7.505	1.00 27.02	D
ATOM	3700	0	VAL I	D	89	101.698	53.772	6.473	1.00 26.22	D
ATOM	3701	N	THR		90	100.530	53.662	8.394	1.00 26.33	D
							54.955	8.219	1.00 26.05	D
ATOM	3702	CA	THR I		90	99.881				
MOTA	3703	CB	THR I		90	98.414	54.802	7.769	1.00 27.24	D
MOTA	3704	OG1	THR I	D	90	98.359	54.063	6.543	1.00 31.41	D
ATOM	3705	CG2	THR I	D	90	97.786	56.163	7.545	1.00 28.57	· D
ATOM	3706	C	THR		90	99.883	55.698	9.546	1.00 24.83	D
						99.542	55.120	10.581	1.00 25.45	D
ATOM	3707	0	THR		90					
ATOM	3708	N	VAL I		91	100.266	56.972	9.512	1.00 22.04	D
ATOM	3709	CA	VAL :	D	91	100.300	57.791	10.716	1.00 21.50	D
MOTA	3710	CB	VAL 1	D	91	101.749	58.280	11.031	1.00 23.04	D
ATOM	3711	CG1	VAL I	D	91	101.737	59.245	12.225	1.00 22.74	D
ATOM	3712		VAL		91	102.650	57.082	11.340	1.00 20.38	D
						99.369	58.993	10.553	1.00 21.65	D
MOTA	3713	C	VAL		91					
ATOM	3714	0	VAL		91	99.357	59.653	9.509	1.00 21.70	D
ATOM	3715	N	PHE	D	92	98.573	59.252	11.586	1.00 21.34	D
ATOM	3716	CA	PHE	D	92	97.633	60.363	11.580	1.00 21.48	D
ATOM	3717	CB	PHE	D	92	96.370	59.985	10.788	1.00 21.60	D
		CG	PHE		92	95.652	58.771	11.314	1.00 22.22	D
ATOM	3718								1.00 24.10	D
MOTA	3719		PHE		92	94.601	58.902	12.215		
MOTA	3720	CD2	PHE	D	92	96.038	57.495	10.925	1.00 24.53	ם
ATOM	3721	CE1	PHE	D	92	93.940	57.774	12.724	1.00 22.72	D
ATOM	3722	CE2	PHE	D	92	95.386	56.355	11.428	1.00 23.87	D
MOTA	3723	cz	PHE		92	94.335	56.501	12.329	1.00 21.18	D
					92	97.303	60.700	13.030	1.00 22.72	D
MOTA	3724	C	PHE						1.00 22.31	Ď
ATOM	3725	0	PHE		92	97.607	59.921	13.933		
MOTA	3726	N	SER	D	93	96.696	61.859	13.261	1.00 22.45	D
ATOM	3727	CA	SER	D	93	96.366	62.262	14.623	1.00 21.69	D
ATOM	3728	СВ	SER		93	96.599	63.764	14.799	1.00 20.96	D
			SER		93	95.696	64.508	14.010	1.00 25.08	D
MOTA	3729	OG							1.00 21.02	D
MOTA	3730	С	SER		93	94.931	61.913	14.990		
ATOM	3731	0	SER	Ð	93	94.078	61.755	14.127	1.00 20.62	D
MOTA	3732	N	LYS	D	94	94.676	61.791	16.283	1.00 20.66	D
ATOM	3733	CA	LYS	D	94	93.350	61.453	16.768	1.00 24.11	ם
ATOM	3734	СВ	LYS		94	93.444	60.985	18.223	1.00 24.91	D
			LYS		94	92.121	60.605	18.865	1.00 29.49	D
MOTA	3735	CG							1.00 32.97	D
ATOM	3736	æ	LYS		94	92.353	60.101	20.293		
MOTA	3737	CE	LYS	D	94	91.050	59.909	21.052	1.00 33.37	D
ATOM	3738	NZ	LYS	D	94	90.175	58.897	20.399	1.00 34.08	D
ATOM	3739	C	LYS	D	94	92.406	62.646	16.654	1.00 24.40	D
ATOM	3740	0	LYS		94	91.224	62.495	16.356	1.00 24.55	D
					95	92.935	63.834	16.894	1.00 25.54	מ
ATOM	3741	N	SER					16.815	1.00 29.22	D
ATOM	3742	CA	SER		95	92.133	65.040			
ATOM	3743	CB	SER	D	95	91.932	65.643	18.208	1.00 30.47	D
ATOM	3744	OG	SER	D	95	91.236	64.746	19.060	1.00 36.11	ם
ATOM	3745	C	SER	D	95	92.843	66.046	15.932	1.00 29.71	D
ATOM	3746	0	SER		95	93.993	65.834	15.531	1.00 29.68	D
ATOM	3747	N	PRO		96	92.159	67.146	15.588	1.00 29.93	D
							67.532	15.843	1.00 31.14	D
MOTA	3748	9	PRO		96	90.760			1.00 29.29	Đ
MOTA	3749	CA	PRO		96	92.836	68.129	14.747		
MOTA	3750	CB	PRO	D	96	91.714	69.097	14.369	1.00 31.65	D
MOTA	3751	CG	PRO	D	96	90.777	69.010	15.545	1.00 30.66	D
MOTA	3752	С	PRO	D	96	93.939	68.765	15.587	1.00 27.35	D
ATOM	3753	ō	PRO		96	93.818	68.904	16.806	1.00 24.86	D
					97	95.025	69.127	14.929	1.00 26.81	D
MOTA	3754	N	VAL				69.706	15.615	1.00 29.25	D
MOTA	3755	CA	VAL		97	96.158				
ATOM	3756	CB	VAL	D	97	97,438	69.501	14.783	1.00 31.49	D
ATOM	3757	CG1	LVAL	D	97	98.652	69.998	15.556	1.00 33.50	D
ATOM	3758	CG2	VAL	D	97	97.583	68.029	14.415	1.00 34.03	D
ATOM	3759	C	VAL		97	96.007	71.196	15.910	1.00 28.80	D
					97	95.749	71.998	15.012	1.00 28.78	D
ATOM	3760	0	VAL					17.178	1.00 27.47	D
MOTA	3761	N	THR		98	96.144	71.559			
MOTA	3762	CA	THR		98	96.091		17.572	1.00 26.55	D
ATOM	3763	CB	THR	D	98	94.723		18.209	1.00 26.16	D
MOTA	3764	OG:	1 THR	D	98	94.684	72.961	19.575	1.00 31.83	D
MOTA	3765		2 THR		98	93.567		17.469	1.00 23.66	D
MOTA	3766	C.	THR		98	97.220		18.581	1.00 25.73	D
MOTA	3767	ō			98	97.260		19.591	1.00 27.12	D
			THR					18.285	1.00 26.12	D
MOTA	3768	N	LEU		99	98.159				D
MOTA	3769	CA	LEU	D	99	99.307	74.236	19.156	1.00 27.47	U

MOTA	3770	CB	LEU D	99	100.089	75.459	18.675	1.00 31.04	D
ATOM	3771	CG	TEA D	99	100.758	75.309 76.607	17.310 16.940	1.00 33.09 1.00 36.20	D D
ATOM ATOM	3772 3773		FEA D	99 99	101.458 101.754	74.165	17.361	1.00 35.56	D
ATOM	3774	c	TEO D	99	98.935	74.416	20.621	1.00 26.08	D
ATOM	3775	0	TEO D	99	98.077	75.222	20.946	1.00 25.97	D
ATOM	3776	N		100	99.585	73.654	21.500	1.00 26.97	D
MOTA	3777	CA	GLY D		99.310	73.749	22.924	1.00 26.03	D D
ATOM	3778	C	GLY D		98.233 98.020	72.798 72.662	23.422 24.629	1.00 26.02 1.00 25.51	D
ATOM ATOM	3779 3780	И	GLY D		97.553	72.002	22.491	1.00 25.73	D
MOTA	3781	CA	GLN D		96.490	71.199	22.820	1.00 28.13	D
ATOM	3782	CB	GLN D	101	95.372	71.297	21.776	1.00 32.24	D
MOTA	3783	CG	GLN D		94.617	69.981	21.560	1.00 38.65	D D
ATOM	3784	CD OE1	GLN D		94.680 95.760	69.459 69.348	20.115 19.511	1.00 41.08	ם
ATOM ATOM	3785 3786	NE2	GLN D		93.515	69.119	19.566	1.00 40.87	D
ATOM	3787	C	GLN D		96.994	69.756	22.861	1.00 25.22	D
ATOM	3788	0	GLN D	101	97.477	69.245	21.857	1.00 24.55	D
MOTA	3789	N	PRO D		96.885	69.078	24.019	1.00 24.18	D D
ATOM	3790	CD	PRO D		96.436 97.359	69.544 67.683	25.343 24.080	1.00 22.22 1.00 22.76	D
MOTA MOTA	3791 3792	CA CB	PRO D		96.983	67.253	25.494	1.00 22.02	D
ATOM	3793	CG	PRO D		97.088	68.542	26.274	1.00 22.44	ם
ATOM	3794	C	PRO D	102	96.649	66.845	23.015	1.00 21.72	D
ATOM	3795	0	PRO D		95.429	66.922	22.876	1.00 22.65 1.00 19.84	D D
MOTA	3796	N	ASN D		97.409 96.833	66.055 65.225	22.264 21.209	1.00 17.89	D
ATOM ATOM	3797 3798	CA CB	ASN D		97.112	65.856	19.838	1.00 16.30	ם
ATOM	3799	CG	ASN D		96.005	65.587	18.824	1.00 16.50	D
MOTA	3800	OD1	ASN D	103	95.552	64.446	18.636	1.00 16.80	D
MOTA	3801	ND2			95.569	66.643	18.160	1.00 14.61 1.00 17.24	D D
ATOM	3802	C O	ASN D		97.410 98.199	63.805 63.473	21.248 22.129	1.00 17.24	D
ATOM ATOM	3803 3804	Ŋ	ILE D		97.010	62.977	20.284	1.00 17.39	D
ATOM	3805	CA	ILE D		97.465	61.595	20.198	1.00 15.30	D
ATOM	3806	CB	IFB D		96.402	60.627	20.755	1.00 17.89	D
ATOM	3807	CG2			96.818	59.175	20.498 22.253	1.00 13.27 1.00 18.46	D D
ATOM	3808 3809		. ILE D		96.202 95.179	60.886 59.965	22.233	1.00 17.98	ā
ATOM ATOM	3810	C.	ILEC		97.760	61.185	18.763	1.00 17.15	Ď
ATOM	3811	0	ILE D		96.887	61.283	17.902	1.00 18.07	D
MOTA	3812	N	LEU D		98.987	60.727	18.509	1.00 16.66	D D
ATOM	3813	CA	LEU		99.370	60.272 60.482	17.177 16.895	1.00 16.59 1.00 17.56	D
ATOM ATOM	3814 3815	CB	TEA D		100.864 101.375	61.926	16.842	1.00 21.66	Ď
ATOM	3816		r Fen i		102.811	61.943	16.302	1.00 21.26	D
MOTA	3817	CD2	FEU I	105	100.460	62.771	15.951	1.00 21.56	D
MOTA	3818	C	LEU I		99.061	58.804	17.128	1.00 17.13 1.00 18.35	D D
MOTA	3819	o N	LEU I		99.368 98.432	58.056 58.399	18.056 16.039	1.00 17.88	D
MOTA MOTA	3820 3821	CA	ILE I		98.045	57.016	15.839	1.00 17.14	D
MOTA	3822	СВ	ILE I		96.525	56.939	15.492	1.00 16.99	D
MOTA	3823		ITE I		96.093	55.496	15.318	1.00 15.63	D
MOTA	3824		l ILE I		95.711	57.619 57.877	16.604 16.260	1.00 19.04 1.00 16.48	D D
ATOM ATOM	3825 3826	CD.	ILE I		94.238 98.876	56.431	14.700	1.00 17.19	D
ATOM	3827	ō	ILE I		98.941	57.004	13.618	1.00 16.06	D
ATOM	3828	N	CYS I		99.540	55.312	14.966	1.00 18.84	D
ATOM	3829	CA	CYS 1		100.339	54.637	13.954	1.00 19.74	D D
MOTA	3830	C	CYS		99.634 99.632	53.323 52.421	13.670 14.507	1.00 20.17 1.00 20.08	D
MOTA MOTA	3831 3832	O CB		D 107	101.755	54.349	14.453	1.00 22.00	D
ATOM	3833	SG		D 107	102.800	53.514	13.211	1.00 28.61	D
MOTA	3834	N	LEU :	D 108	99.027	53.221	12.493	1.00 19.48	מ
MOTA	3835	CA		D 108	98.313	52.015	12.113	1.00 19.67 1.00 19.98	D D
MOTA	3836	CB		D 108	97.024 95.977	52.391 51.358	11.369 10.925	1.00 19.98	D
MOTA MOTA	3837 3838		LEU 1 LEU	D 108	95.883	51.366	9.412	1.00 20.15	D
MOTA	3839		2 LEU		96.301	49.971	11.454	1.00 19.44	D
MOTA	3840	С	LEU	D 108	99.207	51.145	11.237		D
MOTA	3841			D 108	99.657	51.563	10.170		D D
MOTA	3842			D 109	99.473 100.289	49.940 48.972	11.721 11.016		D
MOTA	3843	CA	VAL	D 109	100.203	512			

MOTA	3844	СВ	VAL D 109	101.368	48.402	11.958	1.00 19.40	D
ATOM	3845	CG1	VAL D 109	102.290	47.474	11.202	1.00 18.01	D
ATOM	3846		VAL D 109	102.155	49.560	12.590	1.00 17.30	D
ATOM	3847	C	VAL D 109	99.321	47.876	10.568	1.00 21.45	D
ATOM	3848	0	VAL D 109	98.845	47.079	11.382	1.00 22.65	D
ATOM	3849	N	ASP D 110	99.022 98.086	47.861 46.901	9.274 8.689	1.00 22.00 1.00 23.80	D D
ATOM	3850	CA CB	ASP D 110 ASP D 110	97.156	47.648	7.728	1.00 24.68	D
ATOM ATOM	3851 3852	CG	ASP D 110	95.790	47.002	7.603	1.00 26.64	D
ATOM	3853		ASP D 110	95.582	45.915	8.177	1.00 28.80	D
ATOM	3854		ASP D 110	94.920	47.591	6.926	1.00 27.99	D
ATOM	3855	С	ASP D 110	98.802	45.756	7.944	1.00 23.77	D
ATOM	3856	0	ASP D 110	100.005	45.831	7.684	1.00 22.82	D
ATOM	3857	N	ASN D 111	98.044	44.711	7.604	1.00 23.55	D
MOTA	3858	CA	ASN D 111	98.548	43.530	6.889	1.00 23.79	D
ATOM	3859	CB	ASN D 111	98.880	43.867	5.425	1.00 25.36	D
MOTA	3860	CG	ASN D 111	99.079	42.610	4.562	1.00 29.95 1.00 29.58	D D
ATOM	3861		ASN D 111 ASN D 111	99.981 98.220	42.547 41.611	3.724 4.761	1.00 29.58	ם
MOTA	3862 3863	C ND2	ASN D 111	99.786	42.941	7.556	1.00 22.70	Ď
ATOM ATOM	3864	0	ASN D 111	100.834	42.784	6.929	1.00 22.97	D
ATOM	3865	N	ILE D 112	99.656	42.612	8.835	1.00 22.14	D
ATOM	3866	CA	ILE D 112	100.754	42.038	9.598	1.00 20.20	D
ATOM	3867	СВ	ILE D 112	100.746	42.536	11.055	1.00 18.82	D
ATOM	3868	CG2	ILE D 112	101.926	41.950	11.808	1.00 15.77	D
ATOM	3869	CG1	ILE D 112	100.770	44.058	11.103	1.00 19.09	D
MOTA	3870		ILE D 112	100.630	44.602	12.514	1.00 21.18	D
MOTA	3871	C	ILE D 112	100.666	40.512	9.659	1.00 21.41	D
MOTA	3872	0	ILE D 112	99.626	39.960	10.002	1.00 22.04	D D
ATOM	3873	N	PHE D 113 PHE D 113	101.765	39.838 38.386	9.338 9.409	1.00 21.35 1.00 19.93	D
MOTA MOTA	3874 3875	CA CB	PHE D 113	101.818 100.822	37.726	8.462	1.00 21.28	D
ATOM	3876	CG	PHE D 113	100.537	36.306	8.825	1.00 20.91	D
MOTA	3877		PHE D 113	99.630	36.012	9.838	1.00 19.85	D
ATOM	3878	CD2		101.244	35.261	8.230	1.00 22.61	D
ATOM	3879	CE1	PHE D 113	99.430	34.698	10.264	1.00 20.63	D
ATOM	3880	CE2	PHE D 113	101.054	33.942	8.646	1.00 21.21	D
ATOM	3881	CZ	PHE D 113	100.144	33.660	9.669	1.00 20.87	D
MOTA	3882	C	PHE D 113	103.201	37.871	9.071	1.00 19.98	D
ATOM	3883	0	PHE D 113	103.762	38.238	8.044	1.00 20.80	D
ATOM	3884	N	PRO D 114	103.765	37.005	9.925 9.732	1.00 21.26 1.00 21.94	D D
MOTA	3885	CD.	PRO D 114 PRO D 114	105.101 103.150	36.414 36.518	11.166	1.00 21.41	D
ATOM ATOM	3886 3887	CA CB	PRO D 114	104.117	35.424	11.625	1.00 21.03	D
ATOM	3888	CG	PRO D 114	105.441	35.912	11.115	1.00 22.98	D
ATOM	3889	c	PRO D 114	103.002	37.648	12.185	1.00 21.84	D
ATOM	3890	0	PRO D 114	103.621	38.711	12.034	1.00 20.41	D
ATOM	3891	N	PRO D 115	102.167	37.441	13.222	1.00 22.52	D
ATOM	3892	CD	PRO D 115	101.314	36.256	13.445	1.00 22.08	D
MOTA	3893	CA	PRO D 115	101.937	38.448	14.266	1.00 21.19	D
MOTA	3894	CB	PRO D 115	100.730	37.895	15.025	1.00 20.92	D
ATOM	3895	CG	PRO D 115	100.917 103.139	36.410	14.902 15.171	1.00 19.88 1.00 21.62	D D
MOTA	3896	C	PRO D 115 PRO D 115	103.139	38.683 38.336	16.356	1.00 21.02	D
MOTA MOTA	3897 3898	O N	VAL D 116	104.179	39.263	14.588	1.00 21.58	D
ATOM	3899	CA	VAL D 116	105.405	39.598	15.300	1.00 22.53	D
ATOM	3900	CB	VAL D 116	106.520	38.554	15.067	1.00 24.90	, D
ATOM	3901		VAL D 116	107.817	39.035	15.713	1.00 24.06	D
MOTA	3902	CG2	VAL D 116	106.104	37.195	15.641	1.00 24.88	ם
MOTA	3903	C	VAL D 116	105.855	40.929	14.708	1.00 21.86	D
ATOM	3904	0	VAL D 116	106.114	41.027	13.509	1.00 20.87	D
MOTA	3905	N	VAL D 117	105.935	41.962	15.534	1.00 20.65	D
MOTA	3906	CA	VAL D 117	106.338	43.255	15.007	1.00 21.60 1.00 18.11	D D
MOTA	3907	CB	VAL D 117	105.126	43.978 44.473	14.345 15.403	1.00 16.63	D
ATOM ATOM	3908		L VAL D 117 2 VAL D 117	104.156 105.599	45.101	13.469	1.00 17.02	D
ATOM	3909 3910	CG.	VAL D 117	106.928	44.137	16.092	1.00 23.84	D
ATOM	3911	o	VAL D 117	106.677	43.936	17.280	1.00 24.78	D
ATOM	3912	N	ASN D 118	107.719	45.113	15.670	1.00 27.93	D
ATOM	3913	CA	ASN D 118	108.348	46.051		1.00 30.45	ם
ATOM	3914	СВ	ASN D 118	109.866	45.898	16.538	1.00 33.93	D
ATOM	3915	CG		110.564	46.644		1.00 39.88	D
ATOM	3916		1 ASN D 118	110.327	47.834		1.00 42.45	D
MOTA	3917	ND:	2 ASN D 118	111.438	45.946	18.375	1.00 43.14	D

ATOM	3918	C	ASN D 118	107.960	47.465	16.181	1.00 27.72	D
ATOM	3919	0	ASN D 118	108.398	47.952	15.140	1.00 26.88	D
MOTA	3920	N	ILE D 119	107.126	48.113	16.988	1.00 27.59 1.00 27.12	D D
ATOM	3921	CA	ILE D 119 ILE D 119	106.680 105.133	49.476 49.580	16.700 16.719	1.00 27.12	D
ATOM ATOM	3922 3923	CB	ILE D 119	104.698	50.994	16.346	1.00 26.16	D
ATOM	3924		ILE D 119	104.528	48.572	15.741	1.00 24.63	D
ATOM	3925	-	ILE D 119	103.026	48.423	15.877	1.00 24.19	D
ATOM	3926	C	ILE D 119	107.243	50.436	17.746	1.00 27.72	D
MOTA	3927	0	ILE D 119	107.050	50.248	18.946	1.00 26.86	D
MOTA	3928	N	THR D 120	107.951	51.460	17.291	1.00 27.54	D
ATOM	3929	CA	THR D 120	108.524	52.423	18.214	1.00 29.37	D
MOTA	3930	CB	THR D 120	110.022	52.131	18.477	1.00 32.22	D
MOTA	3931		THR D 120	110.722	52.034	17.229	1.00 35.14 1.00 35.67	D D
ATOM	3932	-	THR D 120 THR D 120	110.176 108.369	50.817 53.826	19.247 17.668	1.00 33.07	D
ATOM ATOM	3933 3934	C C	THR D 120	108.398	54.035	16.459	1.00 29.89	D
ATOM	3935	Ŋ	TRP D 121	108.187	54.789	18.560	1.00 26.28	D
ATOM	3936	CA	TRP D 121	108.031	56.171	18.135	1.00 26.93	D
ATOM	3937	СВ	TRP D 121	106.935	56.866	18.940	1.00 24.20	D
ATOM	3938	CG	TRP D 121	105.568	56.343	18.687	1.00 22.03	D
ATOM	3939	CD2	TRP D 121	104.643	56.826	17.707	1.00 20.30	D
MOTA	3940		TRP D 121	103.454	56.085	17.856	1.00 20.70	D
MOTA	3941		TRP D 121	104.705	57.817	16.717	1.00 17.15	D D
MOTA	3942		TRP D 121	104.929	55.351	19.365 18.875	1.00 21.06 1.00 22.39	D
MOTA	3943		TRP D 121	103.655 102.332	55.190 56.305	17.057	1.00 17.25	D
MOTA	3944		TRP D 121	103.593	58.036	15.924	1.00 17.92	D
ATOM ATOM	3945 3946	CH2		102.419	57.282	16.099	1.00 19.11	D
ATOM	3947	C	TRP D 121	109.319	56.957	18.284	1.00 26.88	D
ATOM	3948	ō	TRP D 121	110.059	56.789	19.251	1.00 27.48	D
ATOM	3949	N	LEU D 122	109.572	57.830	17.321	1.00 29.82	D
ATOM	3950	CA	LEU D 122	110.764	58.658	17.343	1.00 31.91	D
MOTA	3951	CB	LEU D 122	111.664	58.331	16.144	1.00 34.65	D
MOTA	3952	CG	LEU D 122	112.391	56.977	16.112	1.00 37.28 1.00 37.11	D C
ATOM	3953		LEU D 122	113.247	56.828	17.360 16.025	1.00 37.11	D
ATOM	3954	<b>යා</b> 2	LEU D 122 LEU D 122	111.394 110.416	55.840 60.142	17.324	1.00 31.97	D
ATOM ATOM	3955 3956	С 0	LEU D 122	109.619	60.593	16.503	1.00 31.46	D
ATOM	3957	N	SER D 123	111.010	60.889	18.250	1.00 31.03	D
ATOM	3958	CA	SER D 123	110.813	62.331	18.326	1.00 33.04	D
ATOM	3959	CB	SER D 123	110.312	62.745	19.712	1.00 32.42	D
MOTA	3960	OG	SER D 123	110.169	64.154	19.793	1.00 32.43	D
MOTA	3961	C	SER D 123	112.184	62.948	18.062	1.00 33.10	D D
ATOM	3962	0	SER D 123	113.108	62.784	18.860	1.00 33.57 1.00 33.51	ם
MOTA	3963	N	ASN D 124		63.646	16.941 16.553	1.00 36.20	D
MOTA	3964	CA	ASN D 124		64.258 65.392	17.510	1.00 34.61	D
ATOM	3965 3966	CB CG	ASN D 124 ASN D 124		66.512	17.531	1.00 34.17	D
ATOM ATOM	3967		1 ASN D 124		66.764	16.539	1.00 34.73	D
ATOM	3968		2 ASN D 124		67.202	18.660	1.00 35.34	D
ATOM	3969	C	ASN D 124		63.191	16.561	1.00 37.34	D
ATOM	3970	0	ASN D 124	115.747	63.401	17.104	1.00 37.93	D
MOTA	3971	N	GLY D 125		62.039	15.970	1.00 38.73	D
MOTA	3972	CA			60.951	15.910	1.00 39.56	D D
MOTA	3973	С	GLY D 125		60.131	17.183	1.00 40.55 1.00 42.52	D
MOTA	3974	0	GLY D 125		59.054 60.622	17.157 18.291	1.00 40.35	D
ATOM	3975	N	HIS D 126			19.569	1.00 41.15	D
ATOM	3976 3977	CA CB				20.702	1.00 43.51	· D
MOTA MOTA	3978	CG				20.599	1.00 47.67	D
MOTA	3979		2 HIS D 126			20.422	1.00 47.36	D
MOTA	3980		1 HIS D 126			20.694	1.00 49.39	D
MOTA	3981		1 HIS D 126	118.709		20.581	1.00 48.59	D
ATOM	3982		2 HIS D 126	118.140		20.415		D
ATOM	3983	C	HIS D 120			19.907		D D
MOTA	3984		HIS D 120					D
ATOM	3985		SER D 12'			20.438 20.821		D
MOTA	3986							ā
MOTA	3987							Ď
MOTA MOTA	3988 3989		SER D 12					D
MOTA	3990		SER D 12				1.00 38.52	D
MOTA	3991		VAL D 12					ם

ATOM	3992	CA	VAL D 128	109.967	57.800	22.942	1.00 35.00	D
ATOM	3993	СВ	VAL D 128	108.699	58.444	22.358	1.00 33.68	D
ATOM	3994		VAL D 128	107.834	59.001	23.479	1.00 32.31	D
MOTA	3995	CG2	VAL D 128	109.081	59.543	21.383	1.00 32.69	D
MOTA	3996	С	VAL D 128	109.574	56.608	23.790	1.00 34.62 1.00 35.98	D D
MOTA	3997	0	VAL D 128	109.150	55.584 56.743	23.268 25.100	1.00 35.57	D
ATOM	3998	N	THR D 129	109.715 109.393	55.653	26.007	1.00 38.21	D
MOTA	3999 4000	CA CB	THR D 129 THR D 129	110.562	55.410	26.992	1.00 40.63	D
ATOM ATOM	4001		THR D 129	110.184	54.413	27.949	1.00 44.78	D
ATOM	4002		THR D 129	110.929	56.700	27.715	1.00 42.66	Ð
ATOM	4003	c	THR D 129	108.103	55.862	26.799	1.00 36.54	D
ATOM	4004	0	THR D 129	107.359	54.911	27.042	1.00 38.87	D
MOTA	4005	N	GLU D 130	107.833	57.101	27.195	1.00 33.00	<b>D</b> .
ATOM	4006	CA	GLU D 130	106.631	57.401	27.963	1.00 31.03	D
MOTA	4007	CB	GLU D 130	106.935	58.453	29.039	1.00 33.90	D D
MOTA	4008	CG	GLU D 130	108.067	58.089 56.788	29.987 30.731	1.00 38.08 1.00 43.43	Ď
MOTA	4009	CD	GLU D 130	107.809 106.744	56.672	31.375	1.00 45.61	ā
ATOM	4010	OE1		108.671	55.879	30.675	1.00 45.67	D
MOTA MOTA	4011 4012	C	GLU D 130	105.521	57.922	27.058	1.00 27.87	D
ATOM	4013	ō	GLU D 130	105.795	58.527	26.029	1.00 24.56	D
ATOM	4014	N	GLY D 131	104.272	57.692	27.457	1.00 26.29	Ø
ATOM	4015	CA	GLY D 131	103.140	58.166	26.679	1.00 25.19	D
ATOM	4016	C	GLY D 131	102.826	57.304	25.474	1.00 24.46	D
MOTA	4017	0	GLY D 131	102.130	57.725	24.559	1.00 23.65	D
ATOM	4018	N	VAL D 132	103.349	56.089	25.476	1.00 22.83	D D
MOTA	4019	CA	VAL D 132	103.117	55.169	24.379	1.00 23.04 1.00 22.91	D
MOTA	4020	CB	VAL D 132	104.448	54.674 53.538	23.784 22.821	1.00 24.12	D
MOTA	4021		VAL D 132 VAL D 132	104.182 105.164	55.816	23.076	1.00 22.85	D
MOTA	4022 4023	C	VAL D 132	102.326	53.943	24.829	1.00 21.91	D
MOTA MOTA	4023	Ö	VAL D 132	102.535	53.416	25.917	1.00 21.27	D
ATOM	4025	N	SER D 133	101.412	53.499	23.979	1.00 22.08	D
ATOM	4026	CA	SER D 133	100.622	52.307	24.251	1.00 21.07	D
ATOM	4027	CB	SER D 133	99.405	52.637	25.119	1.00 21.95	D
MOTA	4028	OG	SER D 133	98.567	53.595	24.498	1.00 27.01	D
ATOM	4029	C	SER D 133	100.178	51.738	22.908	1.00 21.27	Ď
MOTA	4030	0	SER D 133	100.344	52.369	21.864	1.00 19.82 1.00 20.29	D D
ATOM	4031	N	GLU D 134	99.627	50.538 49.938	22.926 21.689	1.00 24.12	Ď
ATOM	4032	CA	GLU D 134 GLU D 134	99.182 100.370	49.323	20.932	1.00 26.01	D
ATOM	4033 4034	CB	GLU D 134	100.932	48.045	21.532	1.00 30.80	D
ATOM ATOM	4035	CD	GLU D 134	102.080	47.480	20.704	1.00 35.43	D
MOTA	4036		GLU D 134	102.273	46.243	20.702	1.00 36.93	D
ATOM	4037		2 GLU D 134	102.793	48.278	20.057	1.00 37.66	D
MOTA	4038	C	GLU D 134	98.127	48.882	21.955	1.00 22.81	D
MOTA	4039	0	GLU D 134	97.968	48.416	23.081	1.00 22.94	D D
MOTA	4040	N	THR D 135	97.400	48.522	20.908	1.00 21.95 1.00 20.78	ם
MOTA	4041	CA	THR D 135	96.361	47.519 47.625	21.009 19.843	1.00 20.70	Ď
ATOM	4042	CB	THR D 135 1 THR D 135	95.368 96.032	47.262	18.623	1.00 22.24	D
MOTA	4043	OG:	2 THR D 135	94.833	49.046	19.721	1.00 18.01	D
MOTA MOTA	4044 4045	C C	THR D 135	97.037	46.168	20.890	1.00 20.80	D
MOTA	4046	ō	THR D 135	98.259	46.084	20.742	1.00 21.08	D
MOTA	4047		SER D 136	96.234	45.116	20.972	1.00 19.11	ם
ATOM	4048		SER D 136	96.728	43.764	20.790	1.00 16.93	D
ATOM	4049	CB	SER D 136	95.769	42.755	21.428		D
MOTA	4050	OG		95.656		22.831		D D
MOTA	4051		SER D 136	96.665		19.267		D
MOTA	4052		SER D 136	96.325		18.580 18.733		D
MOTA	4053		PHE D 137	97.002 96.896			***	D
MOTA	4054			97.652				D
MOTA MOTA	4055 4056			99.138				D
ATOM	4050		1 PHE D 137	99.792			1.00 20.23	D
ATOM	4058	CD	2 PHE D 137	99.894			1.00 17.79	D
MOTA	4059	CE	1 PHE D 137	101.187				D
MOTA	4060		2 PHE D 137	101.291			1.00 19.39	D
ATOM	4061			101.935				D
MOTA	4062		PHE D 137	95.402				D D
MOTA	4063		PHE D 137	94.823				D
MOTA	4064		LEU D 138	94.786 93.367				D
ATOM	4065	C P	LEU D 138	33.36	26.131	23.002		_

ATOM	4066	СВ	LEU D 138	92.722	44.175	15.678	1.00 21.40	D
ATOM	4067		LEU D 138	92.452	45.087	16.881	1.00 22.42	D
ATOM	4068		LEU D 138	91.889		.18,032	1.00 23.38	D
ATOM	4069		LEU D 138	93.732	45.764	17.301	1.00 28.68	D
ATOM	4070	C	LEU D 138	93.230	41.982	14.593	1.00 20.56	D
ATOM	4071	ō	LEU D 138	93.919	42.244	13.615	1.00 22.27	D
ATOM	4072	N	SER D 139	92.326	41.013	14.586	1.00 20.44	a
ATOM	4073	CA	SER D 139	92.143	40.142	13.427	1.00 19.23	D
ATOM	4074	СВ	SER D 139	91.222	38.986	13.788	1.00 19.74	D
ATOM	4075	OG	SER D 139	89.888	39.443	13.861	1.00 21.32	D
MOTA	4076	C	SER D 139	91.594	40.802	12.168	1.00 19.43	D,
MOTA	4077	0	SER D 139	91.028	41.893	12.210	1.00 19.49	D
ATOM	4078	N	LYS D 140	91.755	40.102	11.050	1.00 18.62	D
ATOM	4079	CA	LYS D 140	91.276	40.553	9.749	1.00 19.20	D
ATOM	4080	CB	LYS D 140	92.437	41.058	8.895	1.00 18.92	D
ATOM	4081	CG	LYS D 140	93.286	42.126	9.554	1.00 19.38	D
ATOM	4082	CD	LYS D 140	93.254	43.393	8.758	1.00 20.95	D
MOTA	4083	CE	LYS D 140	93.833	43.195	7.377	1.00 18.23	D
ATOM	4084	NZ	LYS D 140	93.743	44.457	6.617	1.00 20.40	D
MOTA	4085	С	LYS D 140	90.660	39.339	9.068	1.00 19.16	D
MOTA	4086	0	LYS D 140	91.091	38.217	9.312	1.00 19.77	D
ATOM	4087	N	SER D 141	89.670	39.552	8.207	1.00 21.60 1.00 23.19	D D
ATOM	4088	CA	SER D 141	89.030	38.438	7.507	1.00 23.19	D
MOTA	4089	CB	SER D 141	87.859	38.948	6.653 5.655	1.00 28.69	D
MOTA	4090	OG	SER D 141	88.288	39.858	6.636	1.00 23.26	Ď
ATOM	4091	C	SER D 141	89.989	37.605 36.454	6.327	1.00 23.20	D
MOTA	4092	0	SER D 141 ASP D 142	89.692 91.137	38.159	6.251	1.00 21.38	D
MOTA	4093	N CA	ASP D 142 ASP D 142	92.075	37.387	5.429	1.00 22.54	D
MOTA	4094	CB	ASP D 142	92.834	38.303	4.466	1.00 25.84	D
ATOM	4095 4096	CG	ASP D 142	93.943	39.064	5.143	1.00 29.78	D
MOTA MOTA	4097		ASP D 142	93.760	39.486	6.309	1.00 31.16	D
ATOM	4098		ASP D 142	94.997	39.246	4.500	1.00 34.64	D
MOTA	4099	c	ASP D 142	93.045	36.637	6.336	1.00 22.89	D
ATOM	4100	ō	ASP D 142	94.027	36.037	5.883	1.00 20.54	Ø
ATOM	4101	N.	HIS D 143	92.753	36.700	7.632	1.00 21.06	D
ATOM.	4102	CA	HIS D 143	93.522	36.020	8.659	1.00 19.58	D
MOTA	4103	CB	HIS D 143	93.628	34.534	8.317	1.00 19.03	D
ATOM	4104	CG	HIS D 143	92.295	33.892	8.104	1.00 23.00	D
ATOM	4105	CD2	HIS D 143	91.827	33.108	7.104	1.00 24.78	D
MOTA	4106	ND1	HIS D 143	91.237	34.087	8.967	1.00 21.97	D
ATOM	4107	CE1	HIS D 143	90.174	33.455	8.505	1.00 24.67	D
ATOM	4108	NE2	HIS D 143	90.504	32.853	7.375	1.00 24.72	D
ATOM	4109	C	HIS D 143	94.878	36.602	8.986	1.00 20.11	D
MOTA	4110	0	HIS D 143	95.691	35.962	9.654	1.00 21.09	D
MOTA	4111	N	SER D 144	95.118	37.820	8.514	1.00 21.24	D
ATOM	4112	CA	SER D 144	96.352	38.525	8.826	1.00 21.79	Ď D
MOTA	4113	CB	SER D 144	96.834	39.353	7.627	1.00 20.33 1.00 24.32	D
MOTA	4114	OG	SER D 144	96.047	40.511	, 7.434 9.990	1.00 21.43	D
ATOM	4115	C	SER D 144	95.940	39.440	10.504	1.00 20.74	D
MOTA	4116	0	SER D 144	94.830	39.317 40.352	10.504	1.00 21.56	D
MOTA	4117	N	PHE D 145	96.809 96.463	41.235	11.523	1.00 22.54	Ď
ATOM	4118	CA	PHE D 145 PHE D 145	97.156	40.791	12.817	1.00 22.63	D
MOTA	4119	CB	PHE D 145	96.896	39.368	13.200	1.00 25.73	D
MOTA	4120	CG	PHE D 145	97.565	38.329	12.562	1.00 26.67	D
MOTA	4121 4122		PHE D 145	95.987	39.063	14.207	1.00 23.65	D
ATOM ATOM	4123		PHE D 145	97.333	37.004	12.921	1.00 27.30	D
MOTA	4124		PHE D 145	95.750	37.746	14.572	1.00 25.43	Œ
MOTA	4125	CZ	PHE D 145	96.426	36.713	13.926	1.00 24.90	D
ATOM	4126	c	PHE D 145	96.850	42.687	11.299	1.00 22.51	D
ATOM	4127	ŏ	PHE D 145	97.540	43.028	10.339	1.00 23.97	D
ATOM	4128	N	PHE D 146	96.371	43.540	12.198	1.00 20.96	D
ATOM	4129	•	PHE D 146	96.729	44.946	12.190	1.00 19.68	D
MOTA	4130		PHE D 146	95.696	45.817	11.439	1.00 17.70	D
ATOM	4131	CG	PHE D 146	94.392	46.041	12.159	1.00 15.76	D
MOTA	4132	CD:	1 PHE D 146	94.201	47.173	12.948		D
ATOM	4133	CD:	2 PHE D 146	93.321			1.00 14.70	D
ATOM	4134	CE:	1 PHE D 146	92.961			1.00 13.47	D
ATOM	4135	CE	2 PHE D 146	92.080				D
MOTA	4136		PHE D 146	91.900				D
ATOM	4137		PHE D 146	96.893				D
MOTA	4138	0	PHE D 146	96.373				D
MOTA	4139	N	LYS D 147	97.666	46.379	13.901	1.00 20.23	D

ATOM	4140	CA	LYS D 147	97.910	46.817	15.260	1.00 19.84	D
ATOM	4141	СВ	LYS D 147	99.184	46.148	15.796	1.00 21.50	D
ATOM	4142	CG	LYS D 147	99.651	46.679	17.134	1.00 24.87	D
MOTA	4143	CD	LYS D 147	100.764	45.832	17.724	1.00 27.18	D
ATOM	4144	CR	LYS D 147	100.220	44.515	18.253	1.00 31.41	D
MOTA	4145	NZ	LYS D 147	101.086	43.984	19.341	1.00 32.97	D
ATOM	4146	C	LYS D 147	98.038	48.324	15.274	1.00 18.69	D D
MOTA	4147	0	LYS D 147	98.603	48.914	14.352 16.314	1.00 20.14 1.00 18.22	D
ATOM	4148	N	ILE D 148 ILE D 148	97.497 97.530	48.944 50.387	16.446	1.00 18.25	D
ATOM	4149 4150	CA CB	ILE D 148	96.092	50.942	16.548	1.00 20.80	Ď
ATOM ATOM	4151	CG2	ILE D 148	96.113	52.459	16.659	1.00 22.44	D
ATOM	4152	CG1	ILE D 148	95.308	50.533	15.292	1.00 23.89	D
MOTA	4153	CD1		93.840	50.858	15.314	1.00 24.42	D
ATOM	4154	c	ILE D 148	98.369	50.816	17.646	1.00 19.71	D
MOTA	4155	0	ILE D 148	98.213	50.294	18.757	1.00 17.77	D
ATOM	4156	N	SER D 149	99.284	51.753	17.395	1.00 19.08	D
MOTA	4157	CA	SER D 149	100.173	52.278	18.424	1.00 18.19	D
ATOM	4158	CB	SER D 149	101.633	52.137	17.991	1.00 18.51	D
MOTA	4159	OG	SER D 149	102.518	52.492	19.040	1.00 19.49	D
MOTA	4160	C	SER D 149	99.839	53.744	18.646	1.00 18.14	D
MOTA	4161	0	SER D 149	99.591	54.490	17.693 19.905	1.00 18.17 1.00 16.95	ם ס
ATOM	4162	N	TYR D 150	99.843 99.503	54.155 55.524	20.261	1.00 16.12	Ď
ATOM	4163	CA	TYR D 150 TYR D 150	98.310	55.524	21.213	1.00 15.57	D
ATOM	4164 4165	CB	TYR D 150	97.116	54.750	20.701	1.00 16.81	D
MOTA MOTA	4166		TYR D 150	96.291	55.276	19.709	1.00 14.33	D
ATOM	4167		TYR D 150	95.197	54.554	19.222	1.00 17.50	D
ATOM	4168		TYR D 150	96.819	53.486	21.199	1.00 15.90	D
ATOM	4169	CE2		95.731	52.760	20.719	1.00 18.41	D
ATOM	4170	cz	TYR D 150	94.928	53.297	19.732	1.00 16.27	D
MOTA	4171	OH	TYR D 150	93.868	52.574	19.244	1.00 20.03	D
MOTA	4172	С	TYR D 150	100.650	56.266	20.922	1.00 16.35	D D
MOTA	4173	0	TYR D 150	101.438	55.690	21.669 20.643	1.00 16.95 1.00 16.64	D
ATOM	4174	N	LEU D 151	100.732 101.760	57.558 58.396	21.227	1.00 16.50	Ď
ATOM	4175	CA CB	LEU D 151 LEU D 151	102.849	58.705	20.203	1.00 15.48	D
ATOM ATOM	4176 4177	CG	LEU D 151	103.806	59.825	20.639	1.00 17.55	D
ATOM	4178		LEU D 151	104.641	59.374	21.834	1.00 16.60	D
ATOM	4179		LEU D 151	104.702	60.213	19.476	1.00 16.11	D
ATOM	4180	C	LEU D 151	101.140	59.701	21.693	1.00 17.56	D
ATOM	4181	0	LEU D 151	100.577	60.440	20.888	1.00 17.18	D
ATOM	4182	N	THR D 152	101.233	59.997	22.983	1.00 16.14	D
ATOM	4183	CA	THR D 152	100.690	61.259	23.448	1.00 19.47	D D
ATOM	4184	CB	THR D 152	100.359	61.248 60.871	24.966 25.725	1.00 21.24 1.00 25.03	D
ATOM	4185		THR D 152	101.517 99.214	60.281	25.247	1.00 20.79	D
MOTA	4186	CG2	THR D 152	101.717	62.345	23.151	1.00 19.82	D
MOTA MOTA	4187 4188	ò	THR D 152	102.921	62.113	23.218	1.00 21.31	D
MOTA	4189	N	LEU D 153	101.241	63.523	22.781	1.00 20.76	D
ATOM	4190	CA	LEU D 153	102.143	64.617	22.488	1.00 24.15	D
ATOM	4191	CB	LEU D 153	102.760	64.450	21.089	1.00 25.45	D
MOTA	4192	CG	LEU D 153	101.959	64.575	19.785	1.00 27.17	D
ATOM	4193		L LEU D 153	100.520	64.101	19.986	1.00 27.83	D
MOTA	4194		2 LEU D 153	101.982	66.015	19.319	1.00 27.38	D
MOTA	4195	С	LEU D 153	101.440	65.952	22.601	1.00 25.73 1.00 26.55	D
ATOM	4196	0	LEU D 153	100.208	66.028	22.681 22.640	1.00 26.77	D D
MOTA	4197	N	LEU D 154 LEU D 154	102.251 101.781	67.000 68.369	22.734	1.00 26.34	D
ATOM	4198	CA CB	LEU D 154	102.298	69.027	24.019	1.00 25.08	D
ATOM ATOM	4199 4200	CG	LEU D 154	101.877	70.478	24.288	1.00 26.28	D
ATOM	4201		1 LEU D 154	100.377	70.531	24.570	1.00 24.44	D
ATOM	4202		2 LEU D 154	102.667	71.031	25.477	1.00 23.08	D
ATOM	4203	C	LEU D 154	102.374	69.063	21.522	1.00 28.41	D
MOTA	4204	0	LEU D 154	103.577	69.327		1.00 27.19	D
MOTA	4205	N	PRO D 155	101.534	69.351		1.00 30.32	D
MOTA	4206	CD		100.109	68.979		1.00 30.25	D D
MOTA	4207			101.965	70.014	19.294	1.00 31.71 1.00 31.92	D
MOTA	4208			100.667 99.861	70.160 68.968		1.00 31.52	D
MOTA	4209		PRO D 155 PRO D 155	102.663	71.354		1.00 35.12	D
ATOM ATOM	4210 4211		PRO D 155	102.110				D
ATOM	4212		SER D 156	103.893			1.00 39.00	מ
ATOM	4213			104.706		19.083	1.00 42.94	D

MOTA	4214	СB	SER D	156	105.819	72.492	20.121	1.00 43.03	D
ATOM	4215	OG	SER D	156	105.288	72.385	21.430	1.00 45.30	D
ATOM	4216	C	SER D	156	105.311	72.763	17.694	1.00 46.03	D
ATOM	4217	0	SER D	156	104.875	72.084	16.770	1.00 47.06	D
MOTA	4218	N	ALA D	157	106.316	73.609	17.534	1.00 49.61	D
MOTA	4219	CA	ALA D	157	106.931	73.756	16.222	1.00 51.03	D
MOTA	4220	CB	ALA D	157	106.977	75.231	15.828	1.00 51.20	D
ATOM	4221	C	ALA D	157	108.334	73.163	16.195	1.00 51.50	ם
ATOM	4222	0	ALA D	157	108.985	73.147	15.150	1.00 52.20	ם
ATOM	4223	N	GLU D	158	108.797	72.669	17.339	1.00 52.37	D
ATOM	4224	CA	GLU D	158	110.141	72.103	17.411	1.00 53.43	D
MOTA	4225	CB	GLU D	158	110.946	72.785	18.524	1.00 57.17	D
ATOM	4226	CG	GLU D	158	110.401	72.570	19.934	1.00 61.50	α
ATOM	4227	CD	GLU D	158	109.278	73.529	20.291	1.00 63.75	D
ATOM	4228	OE1	GLU D	158	108.757	73.431	21.425	1.00 63.56	D
MOTA	4229	OE2	GLU D	158	108.922	74.381	19.445	1.00 65.17	D
ATOM	4230	C	GLU D	158	110.190	70.592	17.614	1.00 51.03	D
ATOM	4231	0	GLU D	158	111.103	70.084	18.265	1.00 51.07	D
ATOM	4232	N	GLU D	159	109.219	69.876	17.057	1.00 47.47	D
ATOM	4233	CA	GLU D	159	109.185	68.425	17.193	1.00 46.22	D
MOTA	4234	CB	GLU D	159	108.337	68.013	18.406	1.00 47.11	D
MOTA	4235	CG	GLU D		109.127	67.692	19.671	1.00 48.53	D
ATOM	4236	CD	GLO D		108.268	67.042	20.751	1.00 50.37	D
ATOM	4237	OE1			107.319	67.694	21.238	1.00 50.39	D
MOTA	4238	OE2	GLU D		108.537	65.873	21.112	1.00 50.03	D
MOTA	4239	C	GLU D		108.641	67.714	15.960	1.00 43.84	D
ATOM	4240	0	GLU D		107.515	67.974	15.535	1.00 44.12	D
MOTA	4241	N	SER I		109.443	66.825	15.380	1.00 39.56	D
ATOM	4242	CA	SER I		108.993	66.054	14.229	1.00 37.29	D D
ATOM	4243	СВ	SER I		109.971	66.172	13.055	1.00 37.41	D
ATOM	4244	OG	SER I		111.070	65.298	13.206 14.734	1.00 41.72 1.00 35.08	D
ATOM	4245	C	SER I		108.933 109.754	64.615 64.207	15.557	1.00 33.66	D
ATOM	4246	0 N	SER I		107.961	63.846	14.260	1.00 32.11	D
ATOM	4247 4248	N CA	TYR I		107.828	62.478	14.728	1.00 29.69	D
MOTA MOTA	4249	CB	TYR I		106.550	62.315	15.547	1.00 29.62	D
ATOM	4250	CG	TYR I		106.347	63.349	16.620	1.00 29.33	D
ATOM	4251		TYR I		105.761	64.577	16.327	1.00 31.31	D
ATOM	4252		TYR I		105.513	65.515	17.329	1.00 32.70	D
ATOM	4253	CD2			106.695	63.085	17.937	1.00 30.13	D
ATOM	4254	CE2			106.457	64.013	18.947	1.00 30.43	D
ATOM	4255	CZ	TYR I	161	105.863	65.223	18.638	1.00 31.92	D
MOTA	4256	OH	TYR I	161	105.592	66.128	19.643	1.00 35.12	D
MOTA	4257	C	TYR I	161	107.820	61.441	13.627	1.00 29.60	D
MOTA	4258	0	TYR I	161	107.493	61.728	12.473	1.00 29.45	D
MOTA	4259	N	ASP I	162	108.172	60.221	14.005	1.00 29.35	D
MOTA	4260	CA	ASP I		108.201	59.109	13.075	1.00 30.15	D
ATOM	4261	CB	ASP I		109.618	58.863	12.548	1.00 34.90	D
MOTA	4262	CG	ASP I		110.154	60.016	11.733	1.00 37.70	D
ATOM	4263		ASP I		109.669	60.218	10.597	1.00 40.13	D
MOTA	4264		ASP I		111.061	60.716	12.235	1.00 38.68	D
ATOM	4265	C	ASP I		107.759	57.851	13.784		D
ATOM	4266	0	ASP I		108.010	57.672	14.978	1.00 26.72 1.00 29.31	D D
MOTA	4267	N		163	107.088	56.984	13.039 13.569	1.00 29.59	D
MOTA	4268	CA		D 163	106.684	55.700 54.769	12.902	1.00 28.04	D
MOTA	4269	C		D 163 D 163	107.689 107.822	54.772	11.685	1.00 26.22	D
MOTA	4270 4271	O CB		D 163	105.265	55.326	13.134	1.00 29.11	D
MOTA MOTA	4272	SG		D 163	104.703	53.760	13.878	1.00 34.32	D
ATOM	4273	N		D 164	108.417	54.001	13.699	1.00 29.03	D
ATOM	4274	CA		D 164	109.404	53.072	13.161	1.00 29.67	D
MOTA	4275	CB		D 164	110.730	53.238	13.911	1.00 32.54	D
ATOM	4276	CG		D 164	111.874	52.352	13.416	1.00 34.76	D
ATOM	4277	CD		D 164	113.109	52.528	14.297	1.00 34.79	D
ATOM	4278	CE		D 164	114.254	51.630	13.850	1.00 38.29	D
ATOM	4279	NZ		D 164	115.425	51.702	14.775	1.00 36.58	D
ATOM	4280	C		D 164	108.863	51.651	13.322	1.00 28.94	D
ATOM	4281	0		D 164	108.642	51.189	14.443	1.00 29.32	D
ATOM	4282	N	VAL :	D 165	108.632	50.974	12.197	1.00 27.33	D
MOTA	4283	CA		D 165	108.100	49.618	12.212	1.00 26.58	D
MOTA	4284	CB		D 165	106.797	49.516	11.359	1.00 27.12	D
MOTA	4285		LVAL		106.199	48.122	11.462	1.00 25.56	D
MOTA	4286		VAL		105.787	50.544	11.827	1.00 27.97	D
MOTA	4287	C	VAL	D 165	109.113	48.600	11.690	1.00 26.91	D

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MOTA	4288	0	VAL D 165	109.621	48.720	10.583	1.00 25.56	D
MOTA	4289	N	GLU D 166	109.414	47.606	12.513	1.00 28.75	D
ATOM	4290	CA	GLU D 166	110.338	46.544	12.139	1.00 30.67	Ð
ATOM	4291	СВ	GLU D 166	111.445	46.410	13.194	1.00 33.57	ם
		CG	GLU D 166	112.452	47.565	13.142	1.00 41.68	D
MOTA	4292			113.506	47.526	14.244	1.00 46.12	ם
ATOM	4293	CD	GLU D 166				1.00 49.01	D
MOTA	4294		GLU D 166	114.482	48.304	14.146		
MOTA	4295	OE2	GLU D 166	113.363	46.736	15.206	1.00 49.40	D
MOTA	4296	C	GLU D 166	109.543	45.243	12.008	1.00 30.18	D
ATOM	4297	0	GLU D 166	108.737	44.900	12.878	1.00 28.51	D
ATOM	4298	N	HIS D 167	109.759	44.535	10.907	1.00 29.48	D
		CA	HIS D 167	109.056	43.281	10.648	1.00 30.29	D
ATOM	4299			107.686	43.569	10.025	1.00 29.56	D
MOTA	4300	CB	HIS D 167			9.903	1.00 30.02	D
MOTA	4301	CG	HIS D 167	106.808	42.363			
ATOM	4302		HIS D 167	106.562	41.541	8.856	1.00 29.91	D
ATOM	4303	ND1	HIS D 167	106.068	41.871	10.957	1.00 31.27	D
MOTA	4304	CE1	HIS D 167	105.404	40.798	10.564	1.00 28.43	D
ATOM	4305	NE2	HIS D 167	105.687	40.576	9.293	1.00 28.97	D
ATOM	4306	C	HIS D 167	109.886	42.440	9.684	1.00 30.36	D
		ō	HIS D 167	110.607	42.976	8.842	1.00 30.66	D
ATOM	4307			109.775	41.122	9.801	1.00 31.13	D
MOTA	4308	N	TRP D 168				1.00 32.08	D
ATOM	4309	CA	TRP D 168	110.521	40.219	8.930		
MOTA	4310	CB	TRP D 168	110.270	38.765	9.336	1.00 28.28	D
MOTA	4311	CG	TRP D 168	110.665	38.475	10.739	1.00 26.36	D
ATOM	4312	CD2	TRP D 168	110.031	37.556	11.635	1.00 25.51	D
ATOM	4313	CB2		110.759	37.578	12.842	1.00 26.35	D
	4314	CE3		108.916	36.715	11.534	1.00 24.88	σ
MOTA			TRP D 168	111.721	39.004	11.416	1.00 27.27	D
MOTA	4315				38.471	12.682	1.00 28.25	D
MOTA	4316		TRP D 168	111.786			1.00 27.00	D
ATOM	4317	CZ2		110.412	36.791	13.943		
MOTA	4318	CZ3	TRP D 168	108.568	35.932	12.628	1.00 25.90	D
ATOM	4319	CH2	TRP D 168	109.315	35.976	13.817	1.00 26.65	D
ATOM	4320	C	TRP D 168	110.180	40.403	7.452	1.00 33.22	D
MOTA	4321	ō	TRP D 168	111.011	40.139	6.582	1.00 33.90	D
	4322	N	GLY D 169	108.959	40.853	7.174	1.00 34.75	D
MOTA				108.533	41.060	5.797	1.00 36.14	D
MOTA	4323	CA	GLY D 169			5.215	1.00 37.80	D
MOTA	4324	C	GLY D 169	109.056	42.359			D
MOTA	4325	0	GLY D 169	108.635	42.796	4.139	1.00 36.95	
MOTA	4326	N	LEU D 170	109.979	42.981	5.938	1.00 38.89	D
MOTA	4327	CA	LEU D 170	110.578	44.234	5.509	1.00 40.79	D
ATOM	4328	СВ	LEU D 170	110.212	45.356	6.480	1.00 39.77	D
	4329	CG	LEU D 170	108.745	45.765	6.581	1.00 39.57	D
ATOM			LEU D 170	108.592	46.809	7.671	1.00 38.10	D
ATOM	4330				46.308	5.243	1.00 39.58	D
MOTA	4331		LEU D 170	108.267		5.465	1.00 42.12	D
MOTA	4332	C	LEU D 170	112.092	44.085			
ATOM	4333	0	LEU D 170	112.688	43.506	6.370	1.00 41.54	Ð
ATOM	4334	N	ASP D 171	112.706	44.613	4.411	1.00 45.36	D
MOTA	4335	CA	ASP D 171	114.158	44.559	4.252	1.00 48.35	D
MOTA	4336	СВ	ASP D 171	114.539	44.947	2.820	1.00 50.69	D
		CG	ASP D 171	113.467	45.775	2.137	1.00 52.75	D
MOTA	4337			113.076	46.827	2.689	1.00 54.19	Ø
MOTA	4338		L ASP D 171			1.046	1.00 54.32	D
ATOM	4339		2 ASP D 171	113.012	45.372		1.00 48.43	D
MOTA	4340	C	ASP D 171	114.849	45.485	5.255		
MOTA	4341	0	ASP D 171	115.816	45.090	5.910	1.00 48.29	D
MOTA	4342	N	LYS D 172	114.348	46.715	5.364	1.00 48.92	D
MOTA	4343	CA	LYS D 172	114.883	47.707	6.299	1.00 49.86	D
ATOM	4344	СВ	LYS D 172	115.502	48.898	5.552	1.00 51.58	D
	4345	CG	LYS D 172	116.667	48.566	4.637	1.00 55.86	D
MOTA			LYS D 172	116.203		3.316		D
MOTA	4346							D
ATOM	4347		LYS D 172	115.408				D
MOTA	4348	NZ	LYS D 172	114.946				
ATOM	4349	C	LYS D 172	113.734	48.224			D
MOTA	4350	0	LYS D 172	112.564	48.026	6.833	1.00 48.43	D
MOTA	4351		PRO D 173	114.050	48.885	8.291	1.00 46.54	D
ATOM	4352			115.355			1.00 46.03	D
				112.974				D
MOTA	4353							D
MOTA	4354			113.722				D
MOTA	4355			114.950				D
MOTA	4356	C	PRO D 173	112.180				
ATOM	4357	0	PRO D 173	112.746				D
MOTA	4358		LEU D 174	110.869	50.434			D
MOTA	4359			110.023		. 7.829	1.00 39.96	D
ATOM	4360			108.675			1.00 40.30	D
	4361			107.900				D
MOTA	4201		, 114 D 1/4	_0,.,00				

ATOM	4362	CD1	TEA D	174	106.637	50.397	6.151	1.00 42.25	D
MOTA	4363	CD2	TEA D	174	107.568	52.698	6.448	1.00 42.67	D
MOTA	4364	C	TEA D	174	109.845	52.586	8.753	1.00 39.80	D
MOTA	4365	0	TEA D	174	109.645	52.420	9.955	1.00 39.99	D
MOTA	4366	N	TEA D	175	109.947	53.792	8.200	1.00 38.49	D
ATOM	4367	CA	LEU D	175	109.787	55.016	8.983	1.00 38.04	D
MOTA	4368	CB	TEA D	175	111.095	55.812	9.045	1.00 38.62	D
ATOM	4369	CG	TEA D	175	112.127	55.442	10.113	1.00 38.70	D
ATOM	4370		TEA D	175	111.518	55.648	11.489	1.00 39.24	D
ATOM	4371		LEU D		112.577	54.001	9.936	1.00 40.07	ם
ATOM	4372	C	LEU D		108.712	55.892	8.372	1.00 37.31	D
ATOM	4373	ō	LEU D		108.885	56.432	7.282	1.00 38.54	ם
MOTA	4374	N	LYS D		107.599	56.033	9.076	1.00 35.14	D
MOTA	4375	CA	LYS D		106.511	56.850	8.577	1.00 34.26	D
ATOM	4376	СВ	LYS D		105.175	56.124	8.768	1.00 33.88	D
ATOM	4377	CG	LYS D		104.204	56.325	7.620	1.00 36.72	D
			LYS D		104.829	55.887	6.295	1.00 37.68	ם
MOTA	4378	CD	LYS D		103.820	55.913	5.155	1.00 39.32	D
ATOM	4379				103.020	57.254	4.974	1.00 40.75	D
ATOM	4380	NZ	LYS D		106.523	58.166	9.335	1.00 32.22	D
MOTA	4381	C	LYS D			58.204	10.537	1.00 32.35	Ď
MOTA	4382	0	LYS D		106.272		8.625	1.00 29.85	D
ATOM	4383	И	HIS D		106.825	59.243	9.229	1.00 29.87	D
ATOM	4384	CA	HIS D		106.897	60.563 61.456	8.411	1.00 30.84	D
ATOM	4385	CB	HIS D		107.836		8.979	1.00 30.84	D
ATOM	4386	CG	HIS D		108.014	62.830		-	D
ATOM	4387		HIS D		107.607	64.042	8.529	1.00 32.01	
MOTA	4388		HIS D		108.695	63.067	10.155	1.00 32.16	D
MOTA	4389		HIS D		108.704	64.365	10.402	1.00 30.49	D
ATOM	4390		HIS D		108.051	64.979	9.431	1.00 31.08	D
MOTA	4391	C	HIS I		105.532	61.228	9.332	1.00 29.28	D
MOTA	4392	0	HIS I		104.709	61.121	8.429	1.00 27.97	D
ATOM	4393	N	TRP I		105.295	61.922	10.439	1.00 29.05	D
MOTA	4394	CA	TRP I		104.031	62.617	10.619	1.00 29.38	D
MOTA	4395	CB	TRP I	178	103.518	62.464	12.048	1.00 26.73	D
MOTA	4396	CG	TRP I	178	102.205	63.165	12.243	1.00 27.32	D
MOTA	4397	CD2	TRP I	178	101.939	64.262	13.122	1.00 24.87	D
ATOM	4398	CE2	TRP I	178	100.580	64.608	12.959	1.00 26.97	D
ATOM	4399	CE3	TRP I	178	102.714	64.986	14.033	1.00 26.15	D
MOTA	4400	CD1	. TRP I	178	101.028	62.898	11.599	1.00 26.41	D
MOTA	4401	NE1	TRP I	178	100.050	63.759	12.023	1.00 25.31	D
ATOM	4402	CZ2	TRP I	178	99.980	65.649	13.675	1.00 25.60	D
ATOM	4403	CZ3	TRP I	178	102.118	66.021	14.746	1.00 27.98	D
MOTA	4404	CH2	TRP I	178	100.763	66.340	14.562	1.00 27.02	D
ATOM	4405	С	TRP I	178	104.185	64.100	10.294	1.00 30.33	D
ATOM	4406	0	TRP I	178	104.756	64.824	11.143	1.00 29.85	D
ATOM	4407	OXI	TRP I	178	103.745	64.512	9.193	1.00 32.23	D
MOTA	4408	CB	SER I	3	113.641	35.776	8.019	1.00 59.19	E
ATOM	4409	OG	SER I	3	112.349	35.748	8.608	1.00 59.65	E
ATOM	4410	С	SER I	3	114.352	33.977	9.601	1.00 57.92	E
MOTA	4411	0	SER I	3	114.571	32.945	8.970	1.00 57.45	E
ATOM	4412	N	SER I	E 3	116.055	35.305	8.352	1.00 59.31	E
ATOM	4413	CA	SER I		114.719	35.342	9.020	1.00 58.85	E
MOTA	4414	N	PRO I		113.799	33.958	10.824	1.00 56.65	E
ATOM	4415	CD	PRO 1		113.679	35.092	11.759	1.00 56.20	E
ATOM	4416	CA	PRO		113.403	32.704	11.472	1.00 55.50	B
ATOM	4417	СВ	PRO		113.362	33.086	12.946	1.00 56.49	E
MOTA	4418	CG	PRO		112.870	34.493	12.893	1.00 56.56	E
ATOM	4419	C	PRO		112.046	32.217	10.957	1.00 53.68	B
ATOM	4420	ō	PRO		111.168	33.024	10.648	1.00 54.06	E
MOTA	4421	N	GLU		111.875	30.903	10.855	1.00 51.52	E
ATOM	4422	CA	GLU		110.610	30.360	10.373	1.00 49.69	E
	4423	CB	GLU		110.831	29.007	9.676	1.00 53.42	B
MOTA					111.305	27.867	10.561	1.00 57.99	E
MOTA	4424 4425	CD			111.671	26.626	9.758	1.00 60.86	E
MOTA			1 GLU		110.857	26.196	8.908	1.00 62.41	E
MOTA	4426				110.837	26.077	9.979	1.00 63.42	E
MOTA	4427		2 GLU			30.231	11.525	1.00 45.48	E
MOTA	4428		GLU		109.619	29.644	12.564	1.00 46.07	E
MOTA	4429		GLU			30.800	11.337	1.00 40.87	E
ATOM	4430		ASP				12.363	1.00 36.20	E
MOTA	4431						12.617	1.00 35.53	E
MOTA	4432						13.827	1.00 33.60	B
MOTA	4433						13.864	1.00 34.88	E
MOTA	4434		1 ASP					1.00 33.84	E
ATOM	4435	ÚΩ	2 ASP	E 6	106.089	32.70/	-1./10		~

* MON	4436	~	ASP	E3	6	106.229	29.915	11.938	1.00 33.07	E
ATOM	4436 4437	С 0	ASP		6	105.882	29.867	10.762	1.00 32.95	E
ATOM		и	PHE		7	105.632	29.228	12.906	1.00 31.08	E
ATOM	4438		PHE		7	104.466	28.380	12.669	1.00 29.18	E
ATOM	4439	CA	PHE		7	104.760	26.950	13.116	1.00 31.11	B
MOTA	4440	CB			7	105.833	26.278	12.305	1.00 31.97	E
ATOM	4441	CG	PHE		7	105.544	25.745	11.053	1.00 31.67	E
ATOM	4442						26.200	12.782	1.00 32.49	E
ATOM	4443		PHE		7	107.141		10.282	1.00 32.43	E
ATOM	4444		PHE		7	106.546	25.141	12.023	1.00 33.41	E
ATOM	4445	CE2	PHE		7	108.148	25.602	10.770	1.00 31.62	E
MOTA	4446	CZ	PHE		7	107.850	25.071	13.504	1.00 27.19	E
ATOM	4447	C	PHE		7 7	103.345	28.994 29.151	14.715	1.00 27.13	B
ATOM	4448	0	PHB			103.483 102.238	29.340	12.855	1.00 25.52	E
ATOM	4449	N	VAL		8	101.127	29.998	13.538	1.00 23.97	E
ATOM	4450	CA	VAL VAL		8 8	100.903	31.411	12.949	1.00 22.51	Ē
MOTA	4451	CB	VAL			99.789	32.130	13.703	1.00 20.58	E
MOTA	4452		VAL		8 8	102.205	32.211	13.002	1.00 22.51	B
MOTA	4453	CG2					29.275	13.510	1.00 24.21	B
ATOM	4454	C	VAL		8 8	99.785 99.369	28.736	12.485	1.00 25.26	E
ATOM	4455	0	VAL		9 .	99.096	29.288	14.643	1.00 23.28	B -
ATOM	4456	N	TYR TYR		9	97.786	28.663	14.724	1.00 23.53	B
ATOM	4457	CA CB	TYR		9	97.796	27.505	15.718	1.00 24.07	B
MOTA	4458		TYR		9	96.562	26.640	15.627	1.00 25.27	B
ATOM	4459	CG			9	96.570	25.460	14.889	1.00 27.68	E
MOTA	4460	CD1	TYR		9	95.435	24.658	14.801	1.00 27.67	E
ATOM	4461	CD2	TYR		9	95.384	27.002	16.272	1.00 24.82	B
MOTA	4462	CE2	TYR		9	94.245	26.211	16.191	1.00 25.29	B
MOTA	4463	CZ	TYR		9	94.277	25.040	15.458	1.00 26.82	E
ATOM	4464 4465	OH	TYR		9	93.163	24.240	15.403	1.00 27.65	B
MOTA MOTA	4466	C	TYR		9	96.775	29.707	15.179	1.00 23.14	E
ATOM	4467	o	TYR		9	97.037	30.476	16.106	1.00 23.66	E
ATOM	4468	N	GLN		10	95,622	29.739	14.523	1.00 21.64	E
ATOM	4469	CA	GLN		10	94.582	30.686	14.892	1.00 21.14	E
ATOM	4470	СВ	GLN		10	94.438	31.793	13.843	1.00 20.35	B
ATOM	4471	CG	GLN		10	95.677	32.598	13.529	1.00 19.58	E
ATOM	4472	CD	GLN		10	95.410	33.655	12.461	1.00 18.44	E
ATOM	4473	OE1			10	94.498	34.474	12.593	1.00 19.00	B
MOTA	4474	NE2			10	96.206	33.640	11.400	1.00 18.89	E
ATOM	4475	C	GLN		10	93,232	29.997	15.006	1.00 19.74	E
ATOM	4476	ŏ	GLN		10	92.904	29.113	14.223	1.00 21.71	E
ATOM	4477	N	PHE		11	92.450	30.408	15.991	1.00 19.13	E
ATOM	4478	CA	PHE		11	91.108	29.887	16.145	1.00 16.86	E
ATOM	4479	CB	PHE		11	90.981	28.881	17.271	1.00 16.74	E
ATOM	4480	CG	PHE		11	89.562	28.466	17.517	1.00 18.71	K
MOTA	4481	CD1	PHE	B	11	88.910	27.615	16.626	1.00 21.10	E
ATOM,	4482	CD2	PHE	E	11	88.849	28.985	18.595	1.00 18.11	E
MOTA	4483	CE1	PHE	E	11	87.559	27.290	16.807	1.00 22.40	E
ATOM	4484	CB2	PHE	E	11	87.499	28.671	18.789	1.00 15.75	E
MOTA	4485	CZ	PHE	E	11	86.854	27.826	17.898	1.00 21.25	E
MOTA	4486	C	PHE	B	11	90.218	31.069	16.451	1.00 17.10	E
MOTA	4487	0	PHE	B	11	90.461	31.819	17.406	1.00 13.97	E
MOTA	4488	N	LYS	E	12	89.197	31.241	15.622	1.00 16.07	E
MOTA	4489	CA	LYS	B	12	88.266	32.338	15.789	1.00 16.96	E
MOTA	4490	CB	LYS	E	12	88.308	33.246	14.564	1.00 17.05	E
MOTA	4491	CG	LYS	E	12	89.703	33.748	14.200	1.00 17.57	E
MOTA	4492	CD	LYS	E	12	89.663	34.535	12.888	1.00 18.92	E
ATOM	4493	CE	LYS	E	12	91.018	35.136	12.532	1.00 17.07	E
MOTA	4494	NZ	LYS	E	1.2	90.920	36.063	11.362	1.00 14.26	E
ATOM	4495	С	LYS		12	86.856	31.803	15.987	1.00 17.87	E
ATOM	4496	0	LYS	E	12	86.354	31.039	15.165	1.00 16.82	E
MOTA	4497	N	GL'		13	86.235	32.195	17.098	1.00 18.19	E
MOTA	4498	CA	GL'		13	84.875	31.776	17.391	1.00 19.62	E
MOTA	4499	С	GT.		13	83.991	32.939	17.010	1.00 19.93	E
ATOM	4500	0	GP.		13	83.539	33.695	17.868	1.00 21.65	E
ATOM	4501	N	ME.		14	83.728	33.070		1.00 19.89	E
MOTA	4502	CA	ME'		14	82.947	34.184			E
MOTA	4503	CB	ME.		14	83.430	34.490			B
MOTA	4504	CG		r e	14	84.937				E
MOTA	4505			r e	14	85.587			1.00 20.32	E
MOTA	4506			re	14	85.218				E
MOTA	4507			re	14	81.429				E
MOTA	4508			TE	14	80.859 80.789				E
MOTA	4509	N	CY.	SE	15	00.107				_

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MOTA	4510	CA	CYS	B	15	79.332	35.336	15.418	1.00 22.09	E
MOTA	4511	C	CYS	E	15	78.882	36.495	14.524	1.00 21.39	E
MOTA	4512	0	CYS	B	15	79.393	37.614	14.644	1.00 19.38	E
MOTA	4513	CB	CYS	B	15	78.841	35.616	16.848	1.00 22.10	E
ATOM	4514	SG	CYS	E	15	78.970	34.281	18.094	1.00 26.75	E
ATOM	4515	N	TYR	E	16	77.931	36.229	13.633	1.00 20.94	E
MOTA	4516	CA	TYR	E	16	77.408	37.270	12.752	1.00 21.23	E
MOTA	4517	CB	TYR	E	16	77.548	36.858	11.287	1.00 18.37	E
ATOM	4518	CG	TYR	E	16	78.972	36.574	10.876	1.00 19.23 .	E
MOTA	4519	CD1	TYR	E	16	79.576	35.354	11.178	1.00 18.71	E
ATOM	4520		TYR		16	80.875	35.084	10.789	1.00 18.69	E
ATOM	4521		TYR		16	79.715	37.524	10.178	1.00 20.25	E
MOTA	4522	CE2	TYR		16	81.022	37.270	9.785	1.00 17.18	E
ATOM	4523	CZ	TYR		16	81.595	36.047	10.088	1.00 21.03	E
ATOM	4524	OH	TYR		16	82.872	35.775	9.662	1.00 22.99	E
ATOM	4525	C	TYR		16	75.938	37.543	13.085	1.00 22.17	B
ATOM	4526	0	TYR		16	75.132	36.612	13.199	1.00 21.71	B
ATOM	4527	N	PHE		17	75.607	38.825	13.247	1.00 23.05	E
ATOM	4528	CA	PHE		17	74.254	39.263	13.591	1.00 23.67	E
ATOM	4529	ÇВ	PHE		17	74.261	39.988	14.942	1.00 22.49	B
ATOM	4530	CG	PHE		17	74.813	39.172	16.084	1.00 25.10	B
ATOM	4531		PHE		17	74.007	38.270	16.772	1.00 24.22	E
ATOM	4532		PHE		17	76.140	39.318	16.482	1.00 24.67	E
ATOM	4533		PHE		17	74.516	37.526	17.844	1.00 24.68	E
ATOM	4534	CE2			17	76.656	38.579	17.548	1.00 24.45	E
ATOM	4535	CZ	PHE		17	75.843	37.684	18.228	1.00 24.13	E
ATOM	4536	C	PHE		17	73.673	40.223	12.549	1.00 25.10	E
ATOM	4537	ŏ	PHE		17	74.390	41.034	11.971	1.00 24.65	E
ATOM	4538	N	THR		18	72.365	40.122	12.333	1.00 27.15	E
ATOM	4539	CA	THR		18	71.638	40.983	11.405	1.00 29.69	E
ATOM	4540	CB	THR		18	71.609	40.397	9.978	1.00 29.46	E
ATOM	4541		THR		18	72.949	40.252	9.500	1.00 32.31	E
ATOM	4542	CG2			18	70.863	41.321	9.032	1.00 28.09	E
ATOM	4543	C	THR		18	70.217	41.080	11.950	1.00 31.56	E
	4544	ō	THR		18	69.638	40.071	12.355	1.00 32.09	E
ATOM	4545	N	ASN		19	69.661	42.290	11.969	1.00 33.38	E
ATOM	4546	CA	ASN		19	68.316	42.495	12.497	1.00 35.02	E
ATOM ATOM	4547	CB	ASN		19	67.279	41.755	11.647	1.00 37.99	E
	4548	CG	ASN		19	66.779	42.587	10.489	1.00 42.21	E
MOTA	4549		ASN		19	66.271	43.695	10.687	1.00 47.70	E
ATOM ATOM	4550		ASN		19	66.910	42.063	9.273	1.00 43.13	B
	4551	C	ASN		19	68.264	41.977	13.924	1.00 34.10	E
MOTA	4552	Ö	ASN		19	67.487	41.077	14.233	1.00 34.27	E
ATOM ATOM	4553	N	GLY		20	69.088	42.553	14.795	1.00 33.50	B
MOTA	4554	CA	GLY		20	69.120	42.106	16.175	1.00 33.61	E
ATOM	4555,	C	GLY		20	69.575	40.663	16.175	1.00 33.98	E
MOTA	4556	ŏ	GLY		20	70.580	40.343	15.541	1.00 34.56	E
ATOM	4557	Ŋ	THE		21	68.847	39.789	16.866	1.00 34.08	E
ATOM	4558	CA	THE		21	69.198	38.372	16.897	1.00 35.71	E
ATOM	4559	СВ	THE		21	69.193	37.809	18.335	1.00 37.69	Е
ATOM	4560		L THE		21	67.907	38.026	18.930	1.00 39.78	E
ATOM	4561	CG2			21	70.268	38.480	19.174	1.00 38.05	E
ATOM	4562	c.	THE		21	68.251	37.517	16.050	1.00 35.19	E
ATOM	4563	ŏ	THE		21	68.092	36.324	16.303	1.00 36.08	E
ATOM	4564	N	GLU		22	67.619	38.129	15.052	1.00 34.15	B
ATOM	4565	CA	GLU		22	66.705	37.405	14.176	1.00 34.08	E
ATOM	4566	СВ	GL		22	65.868	38.388	13.354	1.00 33.12	E
MOTA	4567	CG		JE	22	64.781	39.073	14.164	1.00 33.66	E
MOTA	4568	CD CD		JE	22	64.173	40.266	13.451	1.00 35.85	E
ATOM	4569		1 GLI		22	63.865	40.151	12.244	1.00 35.10	E
ATOM	4570		2 GL		22	63.995	41.317	14.105	1.00 38.34	E
ATOM	4571	C.		JE	22	67.523	36.503	13.265	1.00 33.80	E
MOTA	4572	ŏ		JE	22	67.205	35.329	13.092	1.00 34.50	E
ATOM	4573	N		3 E	23	68.574	37.065	12.678	1.00 33.59	E
ATOM	4574	CA		3 E	23	69.467	36.298	11.818	1.00 33.75	E
ATOM	4575	CB		G E	23	69.703	36.996	10.470	1.00 36.33	E
MOTA	4576			GE		68.599	36.815	9.434	1.00 42.06	E
ATOM	4577			GE		67.342	37.577		1.00 47.83	E
ATOM	4578			GE		66.408	37.696		1.00 51.02	B
ATOM	4579			GB		65.349	38.502		1.00 52.66	E
ATOM	4580		1 AR			65.087	39.263		1.00 50.82	Ė
MOTA	4581			GE		64.555	38.555			E
ATOM	4582			GE		70.788	36.177		1.00 30.98	E
MOTA	4583			GE		71.465	37.172			E
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MOTA	4584	N	VAL E	1	24	71.149	34.955	12.909	1.00 28.33	E
MOTA	4585	CA	VAL E	;	24	72.394	34.735	13.621	1.00 25.06	E
MOTA	4586	CB	VAL E	:	24	72.148	34.500	15.129	1.00 22.98	E
ATOM	4587		VAL E		24	73.456	34.106	15.817	1.00 21.05	15
			VAL E		24	71.582	35.762	15.763	1.00 21.04	E
ATOM	4588		VAL I		24	73.144	33.550	13.049	1.00 23.08	B
MOTA	4589	C					32.458	12.914	1.00 24.17	B
MOTA	4590	0	VAL E		24	72.600				E
MOTA	4591	N	ARG I	S	25	74.398	33.778	12.694	1.00 23.02	
MOTA	4592	CA	ARG I	3	25	75.223	32.718	12.156	1.00 23.30	B
ATOM	4593	CB	ARG F		25	75.511	32.930	10.659	1.00 24.06	E
			ARG I		25	76.653	32.044	10.176	1.00 25.99	E
ATOM	4594	CG						8.774	1.00 28.29	R
MOTA	4595	CD	ARG 1		25	76.470	31.478			E
ATOM	4596	ne	ARG I	3	25	76.468	32.502	7.743	1.00 29.69	
MOTA	4597	CZ	ARG I	3	25	76.786	32.287	6.466	1.00 29.57	E
ATOM	4598	NH1	ARG I	3	25	77.145	31.075	6.047	1.00 27.28	B
ATOM	4599	NH2			25	76.733	33.293	5.604	1.00 26.98	E
					25	76.535	32.631	12.916	1.00 22.65	E
ATOM	4600	C	ARG I					13.041	1.00 22.47	E
ATOM	4601	0	ARG I		25	77.261	33,620			B
MOTA	4602	N	LEU :	E	26	76.828	31.444	13.433	1.00 21.04	
ATOM	4603	CA	LEU :	E	26	78.069	31.227	14.152	1.00 21.94	E
ATOM	4604	СВ	LEU :	E	26	77.834	30.338	15.383	1.00 21.37	E
ATOM	4605	CG	LEU		26	79.054	29.778	16.128	1.00 22.89	E
					26	78.723	29.567	17.602	1.00 25.16	E
ATOM	4606		LEU					15.493	1.00 23.51	B
ATOM	4607	CD2	LEU :		26	79.483	28.466			
MOTA	4608	С	LEU	E	26	79.032	30.552	13.193	1.00 21.17	E
MOTA	4609	0	LEU	E	26	78.637	29.674	12.432	1.00 21.77	B
ATOM	4610	N	VAL	В	27	80.285	30.983	13.201	1.00 19.92	E
ATOM	4611	CA	VAL		27	81.278	30.358	12.345	1.00 21.31	B
			VAL		27	81.530	31.166	11.039	1.00 20.44	E
MOTA	4612	CB						10.156	1.00 21.63	E
ATOM	4613		VAL		27	82.524	30.420			E
ATOM	4614	CG2	VAL	Е	27	80.221	31.366	10.275	1.00 20.48	
MOTA	4615	С	VAL	E	27	82.581	30.231	13.112	1.00 21.74	E
MOTA	4616	0	VAL	E	27	83.189	31.228	13.487	1.00 24.11	E
ATOM	4617	N	SER		28	82.994	29.001	13.383	1.00 20.88	B
			SER		28	84.249	28.799	14.084	1.00 21.53	E
MOTA	4618	CA					27.702	15.152	1.00 20.62	E
MOTA	4619	CB	SER		28	84.113			1.00 29.22	E
MOTA	4620	OG	SER	E	28	83.693	26.475	14.598		
ATOM	4621	C	SER	E	28	85.274	28.433	13.006	1.00 21.41	E
ATOM	4622	0	SER	E	28	84.992	27.631	12.105	1.00 19.11	E
ATOM	4623	N	ARG		29	86.450	29.051	13.090	1.00 18.23	B
			ARG		29	87.496	28.838	12.105	1.00 18.45	B
MOTA	4624	CA					30.124	11.287	1.00 16.91	E
MOTA	4625	CB	ARG		29	87.701			1.00 17.70	E
MOTA	4626	CG	ARG	E	29	86.433	30.817	10.810		E
MOTA	4627	CD	ARG	E	29	86.791		10.109	1.00 18.98	
ATOM	4628	NE	ARG	E	29	85.631	32.902	9.705	1.00 20.82	E
ATOM	4629	CZ	ARG	E	29	84.939	32.704	8.586	1.00 22.76	E
			LARG		29	85.285		7.743	1.00 21.05	E
MOTA	4630					83.904		8.309	1.00 20.13	E
MOTA	4631		ARG		29			12.710	1.00 18.44	E
MOTA	4632	C	ARG		29	88.842			1.00 19.35	E
ATOM	4633	0	ARG	E	29	89.401		13.520		
ATOM	4634	N	SER	E	30	89.351		12.315	1.00 18.98	E
ATOM	4635	CA	SER	E	30	90.657	26.788	12.774	1.00 21.70	E
	4636	СВ	SER	E	30	90.619			1.00 22.10	E
MOTA			SER		30	89.718			1.00 27.24	E
MOTA	4637					91.637				E
ATOM	4638		SER		30				1.00 23.56	E
ATOM	4639	0	SER		30	91.509				E
ATOM	4640	N	ILE	В	31	92.611				
MOTA	4641	CA	ILE	E	31	93.560	28.439			E
MOTA	4642		ILE	E	31	93.563	29.997			E
ATOM	4643		2 ILE		31	94.163	30.470	9.545	1.00 19.19	E
			1 ILE		31	92.143		11.043	1.00 24.76	E
MOTA	4644					91.144				E
MOTA	4645		1 ILE		31					E
MOTA	4646		ILE		31	95.013				E
MOTA	4647	, 0	ILE	E	31	95.566				E
MOTA	4648	N E	TYR	E	32	95.629				
ATOM	4645		TYR	E	32	97.030	27.089			E
ATOM	4650					97.27	7 25.755	9.417	1.00 26.61	E
	465					98.73			1.00 29.24	E
MOTA						99.42				E
ATOM	465		1 TYF			100.77			_	E
ATOM	4653		1 TYF							E
MOTA	465		2 TYF			99.42				E
MOTA	465	5 CI	2 TYF	E	32	100.77				
MOTA	465	6 C2	TYF	E	32	101.43				E
ATOM	465					102.76	8 24.28	0 9.522	2 1.00 33.44	E

							0 252	1.00 24.83	B
MOTA	4658	С	TYR E		97.700	28.225	9.353		
MOTA	4659	0	TYR E	32	97.444	28.415	8.164	1.00 25.49	B
MOTA	4660	N	ASN E	33	98.543	28.985	10.045	1.00 24.28	E
ATOM	4661	CA	ASN E	33	99,202	30.146	9.461	1.00 24.25	E
						29.740	8.324	1.00 23.93	E
MOTA	4662	CB	ASN E		100.144				E
MOTA	4663	CG	asn b	33	101.379	29.014	8.834	1.00 25.26	
ATOM	4664	OD1	ASN E	33	102.003	29.439	9.808	1.00 26.40	B
ATOM	4665	ND2	ASN E	33	101.737	27.918	8.181	1.00 25.47	E
					98.114	31.099	8.980	1.00 24.88	E
MOTA	4666	С	asn e						E
MOTA	4667	0	ASN E	33	97.494	31.780	9.799	1.00 25.88	
MOTA	4668	N	ARG E	34	97.864	31.163	7.677	1.00 24.52	E
MOTA	4669	CA	ARG E	34	96.815	32.055	7.194	1.00 26.32	E
					97.385	33.175	6.317	1.00 26.61	E
ATOM	4670	CB	ARG E					1.00 26.37	E
ATOM	4671	CG	ARG E	34	97.999	34.346	7.072		
MOTA	4672	CD	ARG E	34	97.776	35.646	6.304	1.00 28.18	E
MOTA	4673	NE	ARG E	34	97.886	35.429	4.865	1.00 31.86	E
		CZ	ARG E		97.607	36.332	3.931	1.00 33.42	E
ATOM	4674							1.00 35.40	E
ATOM	4675		ARG E		97.197	37.550	4.265		
ATOM	4676	NH2	ARG E	34	97.722	36.003	2.653	1.00 35.29	B
ATOM	4677	C	ARG E	34	95.728	31.333	6.417	1.00 26.98	E
			ARG I		94.896	31.968	5.763	1.00 28.88	E
MOTA	4678	0						1.00 26.13	B
MOTA	4679	N	GLU F	35	95.719	30.010	6.481		
MOTA	4680	CA	GLU E	3 35	94.698	29.27 <del>9</del>	5.759	1.00 27.02	E
ATOM	4681	CB	GLU F	3 35	95.350	28.359	4.720	1.00 31.96	E
			GLU I		96.284	27.301	5.278	1.00 38.52	E
MOTA	4682	CG						1.00 42.24	E
ATOM	4683	CD	GLU I		97.116	26.633	4.192		
ATOM	4684	OEI	GLU I	3 3 5	98.180	27.187	3.832	1.00 44.86	E
MOTA	4685	OE2	GLU I	₹ 35	96.699	25.565	3.690	1.00 43.70	E
		C	GLU I		93.754	28.498	6.671	1.00 25.31	E
MOTA	4686					27.709	7.522	1.00 22.18	E
ATOM	4687	0	GLU 1		94.175				B
MOTA	4688	N	GLU 1	€ 36	92.464	28.756	6.498	1.00 24.46	
MOTA	4689	CA	GLU I	B 36	91.438	28.085	7.272	1.00 24.13	E
ATOM	4690	CB	GLU I		90.085	28.731	7.001	1.00 24.37	B
					88.975	28.295	7.928	1.00 25.26	E
ATOM	4691	CG	GLT 1					1.00 26.01	E
MOTA	4692	CD	GLU :	E 36	87.669	28.991	7.604		
MOTA	4693	OE1	GLU	E 36	87.672	29.847	6.694	1.00 27.25	E
ATOM	4694	ORS	GLU :	E 36	86.646	28.689	8.253	1.00 27.12	E
					91.413	26.630	6.826	1.00 23.40	E
MOTA	4695	С	GLU :					1.00 23.72	E
MOTA	4696	0	GLU :	E 36	91.252	26.347	5.645		
ATOM	4697	N	ILE	E 37	91.576	25.707	7.767	1.00 23.97	E
MOTA	4698	CA	ILE	E 37	91.579	24.294	7.419	1.00 24.33	E
					92.818	23.578	8.019	1.00 24.98	E
MOTA	4699	CB	ILE				7.532	1.00 24.26	E
MOTA	4700		2 ILE		94.096	24.255			
MOTA	4701	CG:	LILE	E 37	92.771	23.616	9.544	1.00 25.10	E
ATOM	4702	CD:	LILE	E 37	93.822	22,742	10.204	1.00 26.49	E
	4703	C	ILE		90.301	23.555	7.836	1.00 23.49	E
MOTA							7.162	1.00 23.62	B
MOTA	4704	0	ILE		89.871				
ATOM	4705	N	VAL	E 38	89.690	23.975	8.936	1.00 25.16	E
ATOM	4706	CA	VAL	E 38	88.465	23.342	9.415	1.00 25.85	B
		СВ	VAL				10.667	1.00 26.44	E
MOTA	4707						10.932	1.00 27.10	E
ATOM	4708		1 VAL						E
MOTA	4709	CG:	2 VAL	E 38	89.980		10.495	1.00 29.59	
MOTA	4710	C	VAL	E 38	87.481	24.428	9.792	1.00 24.45	E
MOTA	4711	ō	VAL			25.471	10.288	1.00 24.36	E
							9.594	1.00 24.90	E
MOTA	4712	N	ARG					1.00 23.66	E
MOTA	4713	CA	ARG				9.904		
ATOM	4714	CB	ARG	E 39	84.975	26.055	8.678	1.00 25.55	E
ATOM	4715	CG	ARG	E 39	83.956	27.174	8.857	1.00 29.11	E
		CD			83.514	27.755	7.515	1.00 29.37	B
MOTA	4716						6.739	1.00 29.70	E
ATOM	4717	NE						1.00 31.37	E
MOTA	4718	ÇZ					5.516		
MOTA	4719	NH	1 ARG	E 39	83.314	28.842	4.930	1.00 33.54	E
ATOM	4720		2 ARG			29.266	4.879	1.00 27.78	E
							10.328		E
MOTA	4721		ARG						E
ATOM	4722	0	ARG				9.853		
MOTA	4723		PHE	E 40	83.147	25.295	11.242		E
MOTA	4724				81.799	24.918	11.655		E
							13.137		E
MOTA	4725						13.514		E
MOTA	4726								E
MOTA	4727	CI	1 PHE	E 4			13.407		
ATOM	4728		2 PHE		79.31	5 25.004	13.875		E
			1 PHE					1.00 17.84	B
ATOM	4729								E
MOTA	4730		2 PHE						E
MOTA	4731	C2	PHE	E 4	0 77.66	1 23.248	14.003	1.00 10.01	2

MOTA	4732	C	PHE	В	40	80.938	26.148	11.395	1.00 21.77	E
MOTA	4733	0		E	40	81.064	27.167	12.071	1.00 20.81	E
MOTA	4734	N	ASP		41	80.067	26.033	10.404 9.995	1.00 21.82 1.00 21.76	e e
ATOM	4735	CA	ASP ASP	E	41 41	79.181 79.190	27.110 27.182	8.470	1.00 22.62	E
ATOM ATOM	4736 4737	CB CG	ASP		41	78.492	28.400	7.929	1.00 23.09	E
MOTA	4738		ASP		41	77.507	28.864	8.546	1.00 22.57	E
ATOM	4739		ASP		41	78.929	28.881	6.861	1.00 25.40	E
MOTA	4740	C	ASP	E	41	77.801	26.713	10.493	1.00 21.43	E
ATOM	4741	0	ASP	E	41	77.277	25.672	10.085	1.00 22.83	E
ATOM	4742	N	SER		42	77.210	27.520	11.369	1.00 19.04 1.00 20.39	E
ATOM	4743	CA	SER		42	75.896 75.399	27.173 28.220	11.895 12.907	1.00 20.33	E
ATOM	4744	CB OG	SER SER		42 42	75.271	29.505	12.323	1.00 24.30	B
MOTA MOTA	4745 4746	C	SER		42	74.891	27.000	10.762	1.00 20.23	E
ATOM	4747	ŏ	SER		42	73.916	26.267	10.910	1.00 18.97	E
ATOM	4748	N	ASP	B	43	75.145	27.660	9.631	1.00 21.77	B
MOTA	4749	CA	ASP	E	43	74.261	27.556	8.470	1.00 24.99	B
ATOM	4750	CB	ASP		43	74.561	28.651	7.439	1.00 26.10 1.00 28.71	e E
MOTA	4751	CG	ASP		43	73.819 73.078	29.947 30.013	7.727 8.737	1.00 28.71	E
ATOM	4752		ASP ASP		43 43	73.076	30.902	6.939	1.00 31.35	E
ATOM ATOM	4753 4754	C	ASP		43	74.378	26.193	7.809	1.00 25.68	E
ATOM	4755	ō	ASP		43	73.424	25.727	7.190	1.00 28.27	E
ATOM	4756	N	VAL		44	75.544	25.558	7.937	1.00 25.47	E
MOTA	4757	CA	VAL	E	44	75.764	24.229	7.362	1.00 23.51	E
ATOM	4758	CB	VAL		44	77.251	24.007	6.964	1.00 24.39 1.00 19.52	E
MOTA	4759		VAL		44	77.456	22.579 24.984	6.491 5.867	1.00 23.79	E
ATOM	4760		VAL VAL		44 44	77.655 75.356	23.154	8.373	1.00 23.25	E
ATOM ATOM	4761 4762	C 0	VAL		44	74.774	22.136	8.005	1.00 22.01	E
MOTA	4763	N	GLY		45	75.683	23.370	9.644	1.00 22.52	E
ATOM	4764	CA	GLY		45	75.292	22.411	10.664	1.00 21.82	E
MOTA	4765	C	GLY	E	45	76.275	21.311	11.001	1.00 22.07	E
MOTA	4766	0	GLY		45	75.982	20.442	11.818	1.00 22.49 1.00 22.18	e
MOTA	4767	N	GLU		46	77.439	21.317 20.295	10.373 10.691	1.00 23.77	E
MOTA	4768	CA	GLU GLU		46 46	78.421 78.147	19.017	9.891	1.00 26.29	E
MOTA MOTA	4769 4770	CB	GLU		46	78.455	19.112	8.411	1.00 28.23	E
ATOM	4771	CD	GLU		46	78.214	17.795	7.677	1.00 32.67	E
ATOM	4772	OE1			46	78.575	17.706	6.482	1.00 33.19	E
MOTA	4773	OE2			46	77.661		8.290	1.00 33.19	E
ATOM	4774	C	GLU		46	79.807	20.839	10.383 9.747	1.00 23.15° 1.00 23.06	E
ATOM	4775	0	GLU		46 47	79.943 80.835	21.880 20.153	10.857	1.00 21.79	E
ATOM	4776	N CA	PHE		47	82.192		10.599	1.00 22.22	E
ATOM MOTA	4777 4778	CB	PHE		47	83.175		11.515	1.00 22.30	E
ATOM	4779	CG	PHE		47	83.058	20.249	12.968	1.00 22.20	E
ATOM	4780	CD	PHE	E	47	83.867		13.508	1.00 19.80	E
MOTA	4781		PHE		47	82.151		13.802	1.00 23.06	e
MOTA	4782		LPHE		47	83.781		14.858 15.157	1.00 18.93 1.00 22.63	8
MOTA	4783		PHE PHE		47 47	82.055 82.872			1.00 20.81	E
MOTA MOTA	4784 4785	CZ C	PHI			82.513			1.00 24.14	E
ATOM	4786	ō	PHI			82.064			1.00 23.25	E
ATOM	4787	N	ARC			83.272			1.00 22.66	E
MOTA	4788	CA	ARC			83.672			1.00 23.86 1.00 23.48	E
MOTA	4789			3 E		82.801			1.00 25.48	E
MOTA	4790			3 E		81.339 81.159				E
MOTA	4791 4792			G E G E		79.74				E
ATOM ATOM	4793			G E		79.03				E
ATOM	4794		1 AR			79.60	21.513	3.498		E
MOTA	4795		2 AR	G E	48	77.76				B
ATOM	4796			G E		85.11				e
MOTA	4797			G E		85.50				E
MOTA	4798			A E A E		85.92 87.31				E
MOTA MOTA	4799 4800			A E		88.10			1.00 22.46	E
MOTA	4801			AE		87.29			1.00 22.04	E
ATOM	4802			AE		86.50	7 21.72			E
MOTA	4803			L F		88.10				E
MOTA	4804			T I		88.13		_		e
ATOM	4805	CE	VA	T I	s 50	88.05	9 25.36	0 4.478	, 1.00 24.14	2

ATOM	4806	CG1	VAL	B	50	88.341	25.408	5.959	1.00 24.71	E
ATOM	4807	CG2	VAL	E	50	89.010	26.268	3.704	1.00 22.47	E
MOTA	4808	C	VAL	Е	50	89.374	23.578	3.098	1.00 23.50	E
MOTA	4809	0	VAL		50	89.485	24.041	1.963	1.00 24.92	E
ATOM	4810	N	THR		51	90.281	22.770	3.650	1.00 24.49	E
MOTA	4811	CA	THR		51	91.492	22.317	2.951	1.00 25.50	E
MOTA	4812	CB	THR		51	92.742	23.198	3.234	1.00 25.69	e e
ATOM	4813		THR		51	93.171	23.007	4.586	1.00 27.89 1.00 23.29	E
ATOM	4814		THR		51	92.443	24.670	2.985	1.00 23.29	E
ATOM	4815	C	THR		51	91.817	20.895	3.420 4.496	1.00 27.35	B
ATOM	4816	0	THR		51	91.387	20.477 20.154	2.617	1.00 27.33	E
ATOM	4817	N	LEU		52 52	92.576 92.949	18.783	2.956	1.00 28.49	E
ATOM	4818	CA	PEO		52 52	93.995	18.259	1.969	1.00 30.33	E
ATOM	4819	CB CG	LEU		52 52	93.536	17.892	0.556	1.00 34.17	E
ATOM ATOM	4820 4821		LEU		52	94.749	17.628	-0.334	1.00 34.41	B
ATOM	4822		LEU		52	92.644	16.668	0.620	1.00 34.30	E
ATOM	4823	C	LEU		52	93.494	18.645	4.374	1.00 28.20	E
MOTA	4824	ō	LEU		52	93.304	17.624	5.027	1.00 29.17	E
ATOM	4825	N	LEU		53	94.179	19.677	4.839	1.00 28.30	E
ATOM	4826	CA	LEU		53	94.766	19.682	6.171	1.00 28.75	E
ATOM	4827	СВ	LEU		53	95.490	21.015	6.387	1.00 30.37	B
ATOM	4828	CG	LEU		53	96.939	21.010	6.882	1.00 32.74	E
MOTA	4829		LEU		53	97.777	20.085	6.008	1.00 31.60	E
ATOM	4830	CD2	LEU	B	53	97.498	22.444	6.854	1.00 30.06	E
ATOM	4831	C	LEU	E	53	93.727	19.464	7.278	1.00 27.82	E
ATOM	4832	0	LEU	E	53	94.027	18.858	8.312	1.00 25.47	E
ATOM	4833	N	GLY	E	54	92.508	19.957	7.059	1.00 27.39	E
MOTA	4834	CA	GLY	E	54	91.466	19.813	8.062	1.00 26.92	E
ATOM	4835	C	GLY	E	54	90.569	18.589	7.949	1.00 28.33	E
MOTA	4836	0	GLY		54	89.725	18.348	8.813	1.00 28.02	B
MOTA	4837	N	LEU		55	90.755	17.801	6.898	1.00 29.28	E
ATOM	4838	CA	FEO		55	89.930	16.620	6.675	1.00 31.43	E
MOTA	4839	CB	LEU		55	90.410	15.885	5.419	1.00 32.39	E
ATOM	4840	CG	LEU		55	89.426	14.934	4.731	1.00 35.68	E
MOTA	4841		LEU		55	88.086	15.627	4.504	1.00 34.41 1.00 35.99	E
ATOM	4842		LEU		55	90.018	14.473	3.406	1.00 33.99	E
MOTA	4843	C	LEU		55	89.865	15.659	7.867 8.312	1.00 32.58	E
MOTA	4844	0	LEU		55	88.778	15.294 15.235	8.402	1.00 31.67	E
ATOM	4845	N	PRO		56 56	91.023 92.411	15.520	8.000	1.00 31.37	E
MOTA	4846	CD	PRO		56	90.986	14.316	9.546	1.00 31.17	E
MOTA	4847 4848	CB	PRO		56	92.459	14.163	9.919	1.00 30.50	E
MOTA MOTA	4849	CG	PRO		56	93.161	14.352	8.611	1.00 31.19	E
ATOM	4850	C	PRO		56	90.158	14.865	10.708	1.00 31.43	E
ATOM	4851	ō	PRO		56	89.250	14.195	11.205	1.00 32.17	E
ATOM	4852	N	ALA		57	90.473	16.086	11.138	1.00 29.94	B
ATOM	4853	CA	ALA	E	57	89.748	16.709	12.244	1.00 28.45	E
ATOM	4854	CB	ALA	E	57	90.314	18.098	12.532	1.00 27.09	B
ATOM	4855	C	ALA	E	57	88.249	16.807	11.960	1.00 27.57	E
MOTA	4856	0	ALA	E	57	87.436	16.466	12.812	1.00 26.57	B
MOTA	4857	N	ALA	E	58	87.899	17.270	10.761	1.00 27.40	E
ATOM	4858	CA	ALF			86.505	17.422	10.349	1.00 28.85	E
ATOM	4859	CB	ALA		58	86.439	18.007	8.939	1.00 27.80	B
MOTA	4860	C	ALΑ			85.726	16.110	10.406	1.00 30.37	E
MOTA	4861	0	ΑL			84.624	16.058	10.954	1.00 29.58	B
ATOM	4862	И	GLU			86.292	15.052	9.837	1.00 32.24	E
MOTA	4863	CA	GL			85.632	13.750	9.845	1.00 35.22 1.00 36.81	E
MOTA	4864	CB	GLU			86.441	12.724	9.049	1.00 40.89	
MOTA	4865	CG	GLU			86.392		7.549 6.805	1.00 44.28	. E
MOTA	4866	CD	GL			87.057		6.955	1.00 45.76	E
MOTA	4867		LGL			88.291 86.342		6.075	1.00 45.12	E
ATOM	4868		2 GLU					11.260	1.00 34.08	В
MOTA	4869	C	GLI			85.441 84.384		11.596	1.00 34.48	E
MOTA	4870	O	TYI GL(			86.466		12.090	1.00 33.21	E
MOTA	4871	n Ca		RE		86.390		13.463	1.00 32.36	E
ATOM ATOM	4872 4873	CB		RE		87.724		14.177		B
ATOM	4874	CG		RE		87.657		15.594		E
MOTA	4875		1 TY			87.543		15.872		E
ATOM	4876		1 TY			87.394		17.173		E
MOTA	4877		2 TY			87.628		16.655		E
MOTA	4878	CE		R E		87.478		17.965	1.00 40.26	E
ATOM	4879	CZ		R E		87.360		18.218	1.00 41.88	E

ATOM	4880	ОН	TYR	E	60	87.198	11.262	19.508	1.00 44.51	E
ATOM	4881	C	TYR	E	60	85.312	13.623	14.275	1.00 32.30	E
ATOM	4882	0	TYR		60	84.430	12.976	14.839	1.00 30.56	E
ATOM	4883	N	TRP		61	85.391	14.950	14.347	1.00 31.42 1.00 31.35	e
ATOM	4884	CA	TRP TRP	e	61 61	84.412 84.744	15.715 17.219	15.112 15.071	1.00 32.78	E
MOTA MOTA	4885 4886	CB CG	TRP	E	61	86.051	17.584	15.748	1.00 35.14	E
ATOM	4887		TRP		61	86.909	18.687	15.425	1.00 37.07	B
ATOM	4888		TRP		61	87.994	18.655	16.331	1.00 37.15	E
MOTA	4889	CE3	TRP	E	61	86.864	19.706	14.458	1.00 39.50	E
ATOM	4890		TRP		61	86.635	16.947	16.809	1.00 35.82	E
MOTA	4891		TRP		61	87.800	17.582	17.163	1.00 35.66	E
ATOM	4892	CZ2			61	89.034	19.602	16.300	1.00 38.95 1.00 41.16	e
ATOM	4893	CZ3	TRP		61 61	87.902 88.971	20.656 20.591	14.427 15.346	1.00 40.81	E
ATOM ATOM	4894 4895	Chz	TRP		61	82.968	15.472	14.653	1.00 29.29	E
ATOM	4896	ō	TRP		61	82.045	15.563	15.458	1.00 29.20	E
ATOM	4897	N	ASN		62	82.772	15.162	13.373	1.00 27.86	E
ATOM	4898	CA	ASN	E	62	81.428	14.902	12.853	1.00 29.09	E
ATOM	4899	CB	asn		62	81.379	15.051	11.331	1.00 29.42	E
MOTA	4900	CG	ASN		62	81.241	16.492	10.893	1.00 31.22	e
ATOM	4901		ASN		62	80.563 81.870	17.288 16.834	11.545 9.772	1.00 29.56 1.00 31.73	E
ATOM ATOM	4902 4903	C C	asn asn		62 62	80.906	13.519	13.220	1.00 28.26	E
ATOM	4904	Ö	ASN		62	79.716	13.242	13.086	1.00 27.48	E
ATOM	4905	Ŋ	SER		63	81.795	12.647	13.672	1.00 27.47	E
ATOM	4906	CA	SER		63	81.381	11.311	14.056	1.00 29.39	E
ATOM	4907	CB	SER	E	63	82.511	10.310	13.803	1.00 28.56	E
ATOM	4908	OG	SER		63	83.607	10.545	14.671	1.00 32.72	E
MOTA	4909	C	SER		63	80.987	11.310	15.534 16.055	1.00 30.11 1.00 31.52	e
ATOM	4910	0	SER		63 64	80.515 81.173	10.297 12.453	16.035	1.00 28.86	E
MOTA MOTA	4911 4912	N CA	GLN		64	80.834	12.604	17.612	1.00 28.28	E
ATOM	4913	CB	GLN		64	81.929	13.379	18.350	1.00 29.50	E
ATOM	4914	CG	GLN		64	83.330	12.787	18.266	1.00 29.72	E
ATOM	4915	CD	GLN	E	64	83.418	11.412	18.888	1.00 32.69	E
MOTA	4916	OE1			64	83.055	10.405	18.267	1.00 35.22	B
MOTA	4917	NE2			64	83.887	11.358	20.128 17.783	1.00 31.92 1.00 28.42	e
ATOM	4918	C 0	GLN.		64 64	79.522 79.525	13.366 14.599	17.703	1.00 27.68	B
ATOM ATOM	4919 4920	N	LYS		65	78.410	12.648	17.926	1.00 27.17	E
MOTA	4921	CA	LYS		65	77.111	13.300	18.097	1.00 29.82	B
ATOM	4922	CB	LYS		65	75.994	12.258	18.253	1.00 31.43	R
ATOM	4923	CG	LYS	E	65	75.479	11.692	16.936	1.00 37.61	E
MOTA	4924	CD	LYS		65	74.801	12.766	16.072	1.00 41.12	E
MOTA	4925	CE	LYS		65	73.489	13.267	16.696 15.861	1.00 44.25 1.00 44.10	e
MOTA	4926	NZ C	LYS		65 65	72.832 77.067	14.322 14.273	19.278	1.00 28.07	E
ATOM ATOM	4927 4928	o	LYS		65	76.406	15.308	19.211	1.00 27.46	E
MOTA	4929	N	ASI		66	77.758	13.938	20.361	1.00 27.40	E
MOTA	4930	CA	ASI		66	77.783	14.809	21.532	1.00 26.85	E
MOTA	4931	CB	ASI	E	66	78.566	14.142	22.670	1.00 26.10	E
ATOM	4932	CG	ASI		66	79.899	13.576	22.212	1.00 29.25	e
ATOM	4933		ASI		66	79.915	12.836	21.205 22.864	1.00 28.95 1.00 31.03	E
MOTA	4934 4935	C C	ASI ASI		66 66	80.929 78.390	13.858 16.174	21.193	1.00 26.21	Ē
MOTA MOTA	4936	ō	ASI		66	77.844	17.215	21.559	1.00 26.58	E
MOTA	4937	N		3 E	67	79.510	16.170	20.478	1.00 26.25	E
ATOM	4938	CA	IL	B E	67	80.164	17.414	20.100	1.00 25.76	E
MOTA	4939	CB		EB	67	81.551		19.477	1.00 27.31	E
MOTA	4940		LL		67	82.261		19.210	1.00 25.90	e
MOTA	4941		IL		67	82.396		20.429 21.844	1.00 28.85 1.00 32.35	B
MOTA	4942		LIL	e e e e	67 67	82.494 79.307			1.00 25.95	E
ATOM ATOM	4943 4944	0		e e	67	79.307			1.00 26.97	E
ATOM	. 4945	И		UE	68	78.775			1.00 26.05	E
ATOM	4946	CA		ÜΕ		77.927		17.113	1.00 26.36	E
MOTA	4947	CB		UΕ	68	77.382			1.00 26.91	B
MOTA	4948	CG		UE		78.154				E E
MOTA	4949		LE			77.389				E
ATOM	4950	CD:	LE LE	UE		78.311 76.760				E
MOTA MOTA	4951 4952	o		UE		76.433				E
ATOM	4953	И		UE		76.134				E

75.000 18.726 19.471 1.00 30.38 ATOM 4954 CA GLUE 69 74.481 17.720 20.508 1.00 34.06 CB GLU E 69 ATOM 4955 19.989 ATOM 4956 CG GLU E 69 73.426 16.742 1.00 40.55 MOTA 4957 CD GLU E 69 72.211 17.444 19.392 1.00 44.43 ATOM 4958 OR1 GLU E 69 71.802 18.505 19.922 1.00 43.73 OE2 GLU E 69 71.656 16.926 18.397 1.00 48.15 ATOM 4959 ATOM 4960 C GLU E 69 75.335 20.034 20.178 1.00 29.17 GLU E 69 74.587 21.009 20.071 1.00 29.71 ATOM 4961 0 MOTA 4962 N ARG E 70 76.453 20.059 20.899 1.00 26.65 CA ARG E 70 76.844 21.262 ATOM 21.620 1.00 25.51 4963 MOTA 4964 CB ARG E 70 78.001 20.965 22.572 1.00 27.14 MOTA 4965 CG ARG E 70 77.711 19.855 23.563 1.00 31.22 CD ARG E 70 78.637 19.934 24.769 1.00 35.11 ATOM 4966 25.440 1.00 39.19 ATOM 4967 NE ARG E 70 78.758 18.647 R 4968 CZ ARG E 70 79.456 17.628 24.956 1.00 41.08 ATOM B 80.096 17.752 ATOM NH1 ARG E 70 23.802 1.00 45.32 4969 NH2 ARG E 70 ATOM 4970 79.511 16.486 25.618 1.00 44.01 E MOTA 4971 C ARG E 70 77.230 22.395 20.677 1.00 24.57 R ARG B 70 76.927 23.557 20.941 1.00 21.44 ATOM 4972 ٥ LYS E 71 77.897 22.057 19.576 1.00 24.56 ATOM 4973 N CA LYS E 71 78.309 23.071 18.612 1.00 24.08 ATOM 4974 MOTA 4975 CB LYS E 71 79.202 22.452 17.534 1.00 25.39 LYS E 71 80.100 23.474 16.852 1.00 29.73 MOTA 4976 CG CD LYS E 71 ATOM 4977 81.067 24.095 17.862 1.00 30.94 CE LYS E 71 NZ LYS E 71 81.905 25.205 17.256 1.00 31.82 R ATOM 4978 18.290 1.00 33.45 MOTA 4979 82.774 25.849 LYS E 71 77.087 23.732 17.960 1.00 22.42 ATOM 4980 C MOTA 4981 0 LYS E 71 77.045 24.951 17.780 1.00 18.65 ARG E 72 17.620 1.00 22.31 76.092 22.919 ATOM 4982 N 74.867 23.419 17.002 1.00 21.44 ATOM 4983 CA ARG E 72 E MOTA 4984 CB ARG E 72 73.984 22.250 16.578 1.00 19.93 Е CG ARG E 72 74.534 21.497 15.407 1.00 21.45 ATOM 4985 ARG E 72 73.779 20.223 15.141 1.00 23.34 Ε MOTA 4986 CD 74.211 19.643 NE ARGE 72 13.877 1.00 24.99 MOTA 4987 Е ATOM 4988 CZ ARG E 72 74.028 18.377 13.522 1.00 27.42 æ 14.344 1.00 25.90 NH1 ARG E 72 73.411 17.533 MOTA 4989 12.341 1.00 25.41 4990 NH2 ARG E 72 74.475 17.955 ATOM ARG E 72 74.093 24.315 ATOM 4991 C 17.961 1.00 21.34 E 4992 ARG E 72 73.336 25.182 17.535 1.00 23.67 E ATOM 0 N ALA E 73 74.293 24.105 19.256 1.00 21.13 4993 ATOM CA ALA E 73 73.610 24.887 20.281 1.00 22.11 ATOM 4994 CB ALA E 73 ATOM 4995 73.476 24.052 21.568 1.00 21.20 4996 ALA E 73 74.347 26.189 20.576 1.00 22.67 ATOM С ATOM 4997 0 ALA E 73 73.773 27.133 21.125 1.00 25.58 E ALA E 74 75.614 26.248 20.195 1.00 22.52 4998 N ATOM CA ALA E 74 76.420 27.432 20.448 1.00 22.20 ATOM 4999 5000 CB ALA E 74 77.830 27.219 19.910 1.00 24.81 E ATOM ALA E 74 19.882 1.00 22.28 5001 75.828 28.722 ATOM C 76.027 ALA E 74 29.796 20.452 1.00 20.24 E ATOM 5002 0 18.770 1.00 21.92 ATOM 5003 N VAL E 75 75.102 28.634 E ATOM 5004 CA VAL E 75 74.519 29.841 18.185 1.00 21.69 ATOM 5005 CB VAL E 75 73.700 29.517 16.890 1.00 22.61 CG1 VAL E 72.488 28.657 17.219 1.00 24.39 5006 75 Е ATOM 16.218 1.00 24.00 MOTA 5007 CG2 VAL E 75 73.270 30.798 E 5008 VAL E 75 73.639 30.558 19.219 1.00 21.26 E ATOM С MOTA 5009 0 VAL E 75 73.464 31.777 19.164 1.00 20.64 ASP E 73.106 29.802 20.171 1.00 20.84 В 5010 N 76 ATOM 21.220 1.00 23.98 ATOM 5011 CA ASP E 76 72.273 30.385 E ATOM 5012 CB ASP E 76 71.022 29.532 21.471 1.00 25.33 E MOTA 5013 CG ASP E 76 70.010 29.605 20.331 1.00 27.46 E 69.807 30.697 19.763 1.00 29.45 5014 OD1 ASP E 76 ATOM 69.398 28.566 20.020 1.00 31.17 ATOM 5015 OD2 ASP E 76 5016 C ASP E 76 73.044 30.525 22.538 1.00 24.46 R ATOM 72.910 31.524 MOTA 5017 ٥ ASP E 76 23.247 1.00 25.64 ARG E 73.846 29.515 22.855 1.00 23.56 5018 N MOTA 77 24.085 1.00 22.99 ATOM 5019 CA ARG E 77 74.627 29.486 MOTA 5020 CB ARG E 77 75.176 28.077 24.279 1.00 26.55 75.848 27.806 25.607 1.00 33.45 MOTA 5021 CG ARG E 77 75.961 26.295 25.825 1.00 37.66 CD ARG E 77 ATOM 5022 NE ARGE 77 MOTA 5023 74.639 25.666 25.883 1.00 40.99 CZ ARG E 77 24.352 25.862 1.00 43.13 ATOM 5024 74.423 5025 NH1 ARG E 77 75.438 23.503 25.782 1.00 43.11 ATOM 25.914 1.00 44.93 MOTA 5026 NH2 ARG E 77 73.183 23.885 75.763 30.509 24.078 1.00 23.23 C ARG E 77 MOTA 5027

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MOTA	5028	0	ARG		77	76.162	31.022	25.129	1.00 23.14	B
ATOM	5029	N	VAL		78	76.275	30.808	22.889	1.00 20.54	B
MOTA	5030	CA	VAL	E	78	77.354	31.767	22.741	1.00 19.56	E
ATOM	5031	CB	VAL	E	78	78.500	31.181	21.891	1.00 19.17	E
ATOM	5032	CG1	VAL	E	78	79.612	32.208	21.724	1.00 17.69	E
MOTA	5033	CG2	VAL	B	78	79.032	29.921	22.541	1.00 19.40	E
ATOM	5034	C	VAL	E	78	76.888	33.075	22.093	1.00 19.95	E
MOTA	5035	0	VAL	E	78	76.786	34.110	22.756	1.00 21.57	E
ATOM	5036	N	CYS	E	79	76.595	33.021	20.799	1.00 17.88	E
ATOM	5037	CA	CYS		79	76.181	34.205	20.059		
ATOM	5038	c	CYS		79	74.967	34.265		1.00 17.48	E
ATOM	5039	ŏ	CYS		79	75.087		20.620	1.00 18.40	B
ATOM	5040	СВ	CYS		79		36.146	20.967	1.00 16.69	E
MOTA						75.946	33.847	18.592	1.00 17.30	E
	5041	SG	CYS		79	77.361	33.071	17.722	1.00 27.04	E
ATOM	5042	N	ARG		80	73.802	34.326	20.717	1.00 17.59	E
MOTA	5043	CA	ARG		80	72.641	35.050	21.240	1.00 20.01	E
ATOM	5044	CB	ARG		80	71.340	34.256	21.032	1.00 20.22	B
ATOM	5045	CG	ARG		80	70.886	34.213	19.584	1.00 22.92	E
ATOM	5046	CD	ARG		80	69.423	33.811	19.439	1.00 23.91	E
ATOM	5047	NB	ARG	E	80	68.972	33.965	18.057	1.00 23.49	E
ATOM	5048	cz	ARG	E	80	69.206	33.089	17.082	1.00 25.16	E
ATOM	5049	NH1	ARG	Е	80	69.884	31.975	17.326	1.00 24.15	E
ATOM	5050	NH2	ARG	E	80	68.778	33.336	15.851	1.00 25.51	E
MOTA	5051	C	ARG	E	80	72.804	35.423	22.716	1.00 20.35	E
ATOM	5052	0	ARG	E	80	72.317	36.464	23.153	1.00 17.98	E
ATOM	5053	N	HIS		81	73.495	34.581	23.479	1.00 21.22	
ATOM	5054	CA	HIS		81	73.717	34.867	24.895	1.00 21.22	E
ATOM	5055	СВ	HIS		81	74.467	33.717	25.572		E
ATOM	5056	CG	HIS		81	74.955	34.046	26.950	1.00 24.38 1.00 26.42	E
ATOM	5057		HIS		81	76.188				E
ATOM	5058		HIS		81	74.122	34.381	27.404	1.00 26.61	E
ATOM	5059		HIS		81	74.819	34.080	28.048	1.00 26.60	E
ATOM	5060		HIS		81		34.420	29.117	1.00 25.75	E
MOTA	5061	C	HIS		81	76.075	34.609	28.754	1.00 26.16	E
ATOM		0				74.531	36.146	25.060	1.00 21.41	B
	5062		HIS		81	74.109	37.076	25.742	1.00 19.84	E
ATOM ATOM	5063	N	ASN		82	75.700	36.188	24.426	1.00 22.13	E
	5064	CA	ASN		82	76.568	37.361	24.535	1.00 21.51	E
ATOM	5065	CB	ASN		82	77.927	37.111	23.864	1.00 18.47	B
ATOM	5066	CG	ASN		82	78.702	35.982	24.515	1.00 18.09	E
ATOM	5067		ASN		82	78.453	35.632	25.669	1.00 19.05	E
ATOM	5068		asn		82	79.656	35.409	23.777	1.00 15.06	E
ATOM	5069	С	asn		82	75.936	38.612	23.949	1.00 20.33	E
ATOM	5070	0	asn		82	76.212	39.716	24.412	1.00 22.84	E
ATOM	5071	N	TYR		83	75.089	38.454	22.940	1.00 19.71	E
ATOM	5072	CA	TYR	E	83	74.454	39.620	22.336	1.00 20.96	B
ATOM	5073	CB	TYR	E	83	73.619	39.211	21.114	1.00 21.58	В
ATOM	5074	CG	TYR	E	83	73.223	40.368	20.218	1.00 22.56	E
MOTA	5075	CD1	TYR	E	83	72.047	41.090	20.439	1.00 23.70	E
ATOM	5076	CB1	TYR	E	83	71.682	42.152	19.593	1.00 25.46	E
MOTA	5077	CD2	TYR	E	83	74.027	40.736	19.140	1.00 22.35	B
MOTA	5078	CE2	TYR	E	83	73.675	41.788	18.297	1.00 24.48	E
ATOM	5079	CZ	TYR	E	83	72.508	42.491	18.523	1.00 26.06	Ē
ATOM	5080	OH	TYR	B	83	72.185	43.524	17.671	1.00 28.63	E
MOTA	5081	C	TYR		83	73.583	40.345	23.363	1.00 21.22	E
ATOM	5082	ō	TYR		83	73.399	41.557	23.276	1.00 21.25	
ATOM	5083	N	GLN		84	73.046	39.606	24.333		E
ATOM	5084	CA	GLN		84				1.00 22.94	E
ATOM	5085	CB	GLN			72.234 71.631	40.226	25.377	1.00 25.07	E
ATOM	5086	CG	GLN		84		39.180	26.324	1.00 25.76	B
ATOM	5087	CD	GLN		84	70.863	38.047	25.653	1.00 30.97	E
ATOM	5088				84	69.889	38.525	24.594	1.00 33.95	E
ATOM			GLN		84	69.055	39.401	24.840	1.00 36.35	B
	5089		GLN		84	69.986	37.940	23.401	1.00 36.25	E
MOTA	5090	C	GLN		84	73.158	41.145	26.174	1.00 25.41	E
ATOM ATOM	5091	0	GLN		84	72.804	42.290	26.473	1.00 27.11	E
	5092	N	LEU		85	74.344	40.637	26.510	1.00 24.17	B
MOTA	5093	CA	LEU		85	75.330	41.413	27.256	1.00 26.47	E
MOTA	5094	CB	LEU		85	76.601	40.590	27.515	1.00 26.91	E
MOTA	5095	CG	LEU		85	76.485	39.202	28.161	1.00 29.65	E
MOTA	5096		LBU		85	77.872	38.735	28.587	1.00 31.29	E
MOTA	5097		LEU		85	75.564	39.247	29.365	1.00 32.27	E
MOTA	5098	C	LEU		85	75.698	42.661	26.459	1.00 26.89	E
ATOM	5099	0	LEU		85	75.762	43.757	27.004	1.00 28.24	E
ATOM	5100	N	GLU		86	75.941	42.484	25.162	1.00 27.39	E
MOTA	5101	CA	GΓΩ	E	86	76.293	43.603	24.295	1.00 28.02	E

MOTA	5102	СВ	GLU		86	76.492	43.126	22.852	1.00 26.60	E
MOTA	5102	CG	GTA		86	77.524	42.026	22.672	1.00 30.65	E
		CD	GLU		86	78.942	42.457	23.024	1.00 31.17	E
ATOM	5104									B
MOTA	5105		GLU		86	79.860	41.612	22.919	1.00 31.68	E
ATOM	5106	OE2	GLU		86	79.139	43.631	23.402	1.00 31.77	
ATOM	5107	C	GLU		86	75.165	44.630	24.327	1.00 27.95	E
ATOM	5108	0	GLU		86	75.407	45.834	24.257	1.00 24.30	E
MOTA	5109	N	LEU		87	73.935	44.130	24.442	1.00 28.96	E
ATOM	5110	CA	Leu		87	72.736	44.962	24.468	1.00 32.20	E
ATOM	5111	CB	TEA	E	87	71.496	44.062	24.423	1.00 32.64	E
MOTA	5112	CG	LEU	E	87	70.506	44.100	23.248	1.00 35.59	E
ATOM	5113	CD1	LEU	E	87	71.101	44.734	21.997	1.00 35.24	E
MOTA	5114	CD2	LEU	E	87	70.071	42.675	22.965	1.00 34.35	E
ATOM	5115	С	LEU	В	87	72.669	45.893	25.686	1.00 33.33	B
ATOM	5116	0	LEU	E	87	71.967	46.902	25.663	1.00 32.52	E
ATOM	5117	N	ARG		88	73.401	45.560	26.745	1.00 35.06	E
ATOM	5118	CA	ARG		88	73.399	46.389	27.948	1.00 37.29	E
MOTA	5119	CB	ARG		88	73.348	45.524	29.215	1.00 39.69	E
ATOM	5120	CG	ARG		88	72.471	44.275	29.158	1.00 43.37	E
ATOM	5121	CD	ARG		88	72.441	43.592	30.529	1.00 45.38	E
ATOM	5122	NE	ARG		88	71.846	42.257	30.499	1.00 48.76	E
		CZ	ARG		88	70.625	41.985	30.047	1.00 50.95	B
MOTA	5123		ARG			69.854	42.958	29.579	1.00 52.23	E
ATOM	5124				88			30.064	1.00 51.26	E
ATOM	5125		ARG		88	70.171	40.738		1.00 37.36	E
ATOM	5126	C	ARG		88	74.670	47.225	28.010		E
ATOM	5127	0	ARG		88	74.842	48.044	28.913	1.00 37.55	
MOTA	5128	N	THR		89	75.564	47.019	27.049	1.00 36.40	E
MOTA	5129	CA	THR		89	76.834	47.731	27.055	1.00 34.93	E
ATOM	5130	CB	THR		89	77.951	46.807	27.590	1.00 36.26	B
ATOM	5131	001			89	77.973	45.590	26.825	1.00 34.21	E
ATOM	5132	CG2	THR	E	89	77.708	46.478	29.056	1.00 33.95	E
MOTA	5133	C	THR	E	89	77.294	48.304	25.718	1.00 33.37	B
ATOM	5134	0	THR	E	89	76.958	49.431	25.356	1.00 33.30	E
ATOM	5135	N	THR	E	90	78.080	47.510	25.000	1.00 32.11	E
MOTA	5136	ÇA	THR	E	90	78.639	47.895	23.712	1.00 30.45	E
ATOM	5137	СВ	THR		90	79.313	46.681	23.041	1.00 31.20	E
ATOM	5138	OG1			90	80.238	46.086	23.958	1.00 32.67	E
ATOM	5139	CG2			90	80.076	47.109	21.811	1.00 32.64	E
ATOM	5140	c	THR		90	77.639	48.504	22.738	1.00 28.40	E
ATOM	5141	ō	THR		90	77.903	49.538	22.133	1.00 27.20	E
ATOM	5142	N	LEU		91	76.489	47.864	22.582	1.00 29.83	E
ATOM	5143	CA	LEU		91	75.482	48.361	21.655	1.00 29.52	E
			LEU		91	74.474	47.252	21.354	1.00 27.50	E
MOTA	5144	CB						20.550	1.00 27.30	E
MOTA	5145	CG	LEU		91	75.091	46.101			E
ATOM	5146		TEU		91	74.102	44.959	20.457	1.00 24.51 1.00 23.04	E
ATOM	5147	CD2			91	75.487	46.593	19.157		E
MOTA	5148	C	LEU		91	74.770	49.629	22.129	1.00 30.74	
MOTA	5149	0	LEU		91	73.994	50.228	21.382	1.00 31.46	E
ATOM	5150	N	GLN		92	75.035	50.043	23.366	1.00 29.33	E
MOTA	5151	CA	GLN		92	74.427	51.259	23.884	1.00 30.04	E
MOTA	5152	CB	GLN	E	92	73.869	51.044	25.294	1.00 31.55	E
ATOM	5153	CG	GLN	B	92	72.500	50.381	25.327	1.00 36.90	E
MOTA	5154	CD	GLN	E	92	71.865	50.426	26.706	1.00 41.59	E
ATOM	5155	OE1	GLN	E	92	70.760	49.920	26.911	1.00 43.76	B
ATOM	5156	NE2	GLN	E	92	72.563	51.037	27.662	1.00 43.75	B
ATOM	5157	С	GLN	E	92	75.430	52.409	23.898	1.00 28.45	E
ATOM	5158	0	GLN	E	92	75.059	53.558	24.125	1.00 28.57	B
ATOM	5159	N	ARG	E	93	76.699	52.098	23.650	1.00 26.37	E
MOTA	5160	CA	ARG		93	77.737	53.127	23.633	1.00 26.74	E
ATOM	5161	CB	ARG		93	79.112	52.513	23.340	1.00 24.84	E
ATOM	5162	CG	ARG		93	80.260	53.525	23.217	1.00 20.15	E
ATOM	5163	CD	ARG		93	81.569	52.801	22.894	1.00 20.06	E
MOTA	5164	NE	ARG		93	82.718	53.685	22.729	1.00 15.27	E
						83.316	54.330	23.729	1.00 16.93	E
MOTA	5165	CZ	ARG		93		54.197	24.973	1.00 17.82	B
MOTA	5166		ARG		93	82.875		24.973	1.00 17.82	E
MOTA	5167		ARG		93	84.367	55.101		1.00 16.28	E
MOTA	5168	C	ARG		93	77.428	54.173	22.576		E
MOTA	5169	0	ARG		93	77.202	53.847	21.407	1.00 29.80	
MOTA	5170	N	ARG		94	77.411	55.431	22.995	1.00 28.24	E
MOTA	5171	CA	ARG		94	77.159	56.529	22.084	1.00 29.74	E
MOTA	5172	CB	ARG		94	75.661	56.855	22.053	1.00 32.88	E
ATOM	5173	CG	ARG		94	74.912	55.941	21.086	1.00 36.76	E
MOTA	5174	CD	ARC		94	73.402	56.055	21.163	1.00 40.38	E
MOTA	5175	NE	ARG	E	94	72.75B	55.304	20.080	1.00 44.16	E

3.0004		an	220	-	0.4	72.871	53.991	19.894	1 00 42 57	-
ATOM	5176	CZ	ARG		94				1.00 43.57	E
MOTA	5177		ARG		94	73.602	53.259	20.720	1.00 45.04	B
MOTA	5178	NH2	ARG		94	72.262	53.408	18.869	1.00 45.75	B
ATOM	5179	С	ARG	Е	94	77.992	57.734	22.497	1.00 29.26	E
MOTA	5180	0	ARG	B	94	77.773	58.331	23.546	1.00 30.32	E
MOTA	5181	N	VAL	B	95	78.974	58.063	21.667	1.00 26.76	E
ATOM	5182	CA	VAL		95	79.859	59.188	21.936	1.00 25.75	E
ATOM	5183	СВ	VAL		95	81.340	58.763	21.855	1.00 22.33	E
										E
ATOM	5184		VAL		95	82.244	59.914	22.287	1.00 19.80	
MOTA	5185	CG2	VAL		95	81.565	57.534	22.717	1.00 19.11	E
MOTA	5186	C	VAL	E	95	79.600	60.266	20.902	1.00 26.51	E
ATOM	5187	0	VAL	K	95	79.787	60.042	19.703	1.00 27.04	E
ATOM	5188	N	GLU	B	96	79.160	61.430	21.366	1.00 27.28	B
ATOM	5189	CA	GLU		96	78.870	62.536	20.466	1.00 28.16	E
						78.260		21.227	1.00 30.40	E
MOTA	5190	CB	GLU		96		63.716			
MOTA	5191	CG	GLU		96	76.965	63.396	21.952	1.00 34.36	B
ATOM	5192	CD	GLU	E	96	76.348	64.625	22.609	1.00 36.84	E
MOTA	5193	OE1	GLU	Е	96	75.295	64.478	23.272	1.00 38.81	B
MOTA	5194	OE2	GLU	E	96	76.914	65.734	22.460	1.00 35.73	E
MOTA	5195	C	GLU	В	96	80.148	62.987	19.793	1.00 25.65	B
MOTA	5196	ō	GLU		96	81.176	63.171	20.440	1.00 24.93	E
			PRO		97	80.101	63.168	18.473	1.00 25.41	E
ATOM	5197	N								
MOTA	5198	CD	PRO		97	78.977	62.979	17.539	1.00 24.36	B
ATOM	5199	CA	PRO	В	97	81.304	63.603	17.770	1.00 24.81	E
MOTA	5200	CB	PRO	Е	97	80.927	63.416	16.306	1.00 24.85	E
MOTA	5201	CG	PRO	В	97	79.456	63.717	16.309	1.00 25.36	E
ATOM	5202	С	PRO	E	97	81.643	65.048	18.089	1.00 24.48	E
ATOM	5203	ō	PRO		97	80.761	65.844	18.419	1.00 23.85	E
ATOM	5204	N	THR		98	82.927	65.377	18.025	1.00 22.82	E
									1.00 24.12	E
ATOM	5205	CA	THR		98	83.340	66.748	18.244		
MOTA	5206	CB	THR		98	84.679	66.852	19.019	1.00 26.31	E
MOTA	5207	0G1	THR		98	85.744	66.355	18.205	1.00 34.47	E
MOTA	5208	CG2	THR	E	98	84.623	66.049	20.302	1.00 23.83	B
MOTA	5209	C	THR	E	98	83.519	67.254	16.817	1.00 22.12	B
ATOM	5210	0	THR	E	98	84.162	66.601	15.993	1.00 21.35	E
MOTA	5211	N	VAL		99	82.923	6B.400	16.516	1.00 21.99	E
MOTA	5212	CA	VAL		99	83.001	68.957	15.177	1.00 20.67	B
MOTA	5213	CB	VAL		99	81.585	69.217	14.619	1.00 19.57	E
ATOM	5214		VAL		99	81.667	69.645	13.154	1.00 14.62	E
ATOM	5215	CG2	VAL	E	99	80.732	67.944	14.766	1.00 15.20	E
ATOM	5216	C	VAL	K	99	83.814	70.240	15.158	1.00 22.05	E
MOTA	5217	0	VAL	E	99	83.524	71.194	15.884	1.00 22.27	E
ATOM	5218	N	THR		100	84.827	70.250	14.304	1.00 21.34	E
ATOM	5219	CA	THR		100	85.728	71.376	14.176	1.00 23.10	E
							71.024	14.786	1.00 24.55	E
MOTA	5220	CB	THR			87.104				
MOTA	5221		THR			86.941	70.728	16.180	1.00 30.47	E
MOTA	5222	CG2	THR	E	100	88.079	72.183	14.634	1.00 27.79	E
MOTA	5223	С	THR	E	100	85.934	71.777	12.722	1.00 23.36	E
MOTA	5224	0	THR	Е	100	86.024	70.926	11.842	1.00 21.77	E
ATOM	5225	N	ILE			86.009	73.082	12.473	1.00 24.40	E
ATOM	5226	CA	ILE			86.236	73.584	11.124	1.00 25.31	E
							74.518	10.645	1.00 24.21	E
ATOM	5227	CB	ILE			85.092				
ATOM	5228		ILE			85.398	75.044	9.245	1.00 22.51	E
MOTA	5229		ILE			83.760	73.768	10.636	1.00 24.86	E
MOTA	5230	CD1	IFE	B	101	82.584	74.635	10.197	1.00 25.22	B
MOTA	5231	C	ILE	K	101	87.538	74.372	11.116	1.00 26.66	B
MOTA	5232	0	ILE	B	101	87.859	75.065	12.074	1.00 26.18	E
ATOM	5233	N	SER	B	102	88.287	74.262	10.029	1.00 31.17	E
MOTA	5234	CA			102	89.547	74.977	9.902	1.00 35.36	B
ATOM	5235				102	90.619	74.306	10.755	1.00 34.20	E
		CB								E
MOTA	5236	OG			102	90.777	72.953	10.374	1.00 40.09	
MOTA	5237	С	SER	В	102	89.976	74.979	8.448	1.00 36.82	E
MOTA	5238	0	SER	E	102	89.913	73.953	7.777	1.00 36.68	B
ATOM	5239	N	PRO	E	103	90.404	76.139	7.932	1.00 39.96	E
MOTA	5240	CD			103	90.458	77.473	8.553	1.00 40.07	E
ATOM	5241	CA			103	90.831	76.190	6.532	1.00 42.01	E
ATOM	5242				103	90.856	77.682	6.237	1.00 41.76	E
		CB					78.258		1.00 42.86	E
MOTA	5243	CG			103	91.282		7.556		
MOTA	5244	C			103	92.196	75.534	6.390	1.00 44.62	E
MOTA	5245	0			103	92.943	75.430	7.365	1.00 44.53	E
ATOM	5246	N	SER	E	104	92.514	75.086	5.181	1.00 47.92	E
ATOM	5247	CA	SER	E	104	93.789	74.426	4.920	1.00 50.83	E
ATOM	5248	СВ			104	93.712	73.637	3.612	1.00 52.33	E
ATOM	5249	OG			104	94.904	72.901	3.396	1.00 55.60	E

ATOM	5250	C	SER	E	104	94.941	75.422	4.845	1.00	52.18	E
ATOM	5251	0	SER	E	104	96.080	75.093	5.186	1.00	53.53	E
ATOM	5252	N	ASN	E	113	90.669	78.112	-1.692		48.40	B
MOTA	5253	CA	ASN	E	113	90.651	77.795	-0.269		47.57	E
ATOM	5254	CB	ASN	Е	113	89.863	78.854	0.496		51.34	Ē
ATOM	5255	CG	ASN	E	113	90.504	80.219	0.417		52.99	B
MOTA	5256	OD1	ASN	E	113	90.693	80.765	-0.670		55.11	E
ATOM	5257		ASN			90.845	80.781	1.572		55.09	E
ATOM	5258	C			113	90.045	76.424	-0.001		44.87	
ATOM	5259	ō			113	89.374	75.852				E
ATOM	5260	N	LEU					-0.860		44.99	E
ATOM	5261	CA	LEU			90.282	75.904	1.197		41.65	B
ATOM						89.765	74.592	1.568		38.53	E
	5262	CB	LEU			90.823	73.521	1.287		38.84	B
ATOM	5263	CG	LEU			90.383	72.060	1.441		40.32	· E
MOTA	5264		LEU			89.314	71.726	0.400		39.94	E
ATOM	5265		LEU			91.586	71.145	1.266	1.00	40.52	B
ATOM	5266	C	LEU			89.349	74.523	3.036	1.00	34.78	E
ATOM	5267	0	TEO			90.173	74.684	3.929	1.00	33.51	E
ATOM	5268	N	TEA			88.063	74.293	3.278	1.00	32.05	E
ATOM	5269	CA	TEA	Е	115	87.550	74.181	4.641	1.00	29.68	E
ATOM	5270	CB	<b>LEU</b>	E	115	86.158	74.809	4.754	1.00	29.84	E
ATOM	5271	CG	LEU	E	115	86.046	76.257	5.241	1.00	31.52	E
MOTA	5272	CD1	LEU	E	115	87.101	77.140	4.574		32.51	E
ATOM	5273	CD2	LEU	B	115	84.636	76.762	4.948		30.75	E
ATOM	5274	С	LEU	E	115	87.472	72.712	5.034		27.57	E
ATOM	5275	0	LEU			86.871	71.900	4.331		25.33	E
ATOM	5276	N	VAL	E	116	88.089	72.381	6.161		26.32	E
ATOM	5277	CA	VAL			88.099	71.014	6.651		24.42	В
ATOM	5278	CB	VAL			89.513	70.572	7.075		24.51	E
ATOM	5279		VAL			89.467	69.160	7.641			
ATOM	5280		VAL			90.458	70.643			22.66	E
ATOM	5281	C	VAL			87.195		5.879		26.70	E
ATOM	5282	Ö	VAL				70.842	7.846		22.77	E
ATOM						87.376	71.496	8.868		23.04	E
	5283	N	CYS			86.208	69.968	7.717		22.34	E
ATOM	5284	CA	CYS			85.326	69.711	8.840		21.65	B
ATOM	5285	C	CYS			85.769	68.391	9.466		19.44	E
ATOM	5286	0	CYS		117	85.607	67.319	8.877		18.95	E
ATOM	5287	СВ	CYS			83.863	69.626	8.401	1.00	22.57	E
MOTA	5288	SG	CYS			82.771	69.420	9.844	1.00	25.79	E
ATOM	5289	N	SER			86.355	68.488	10.654	1.00	19.92	E
MOTA	5290	CA	SER			86.837	67.330	11.387	1.00	17.98	E
ATOM	5291	CB	SER	E	118	88.115	67.671	12.146	1.00	18.33	E
MOTA	5292	OG	SER	E	118	89.121	68.117	11.260	1.00	24.58	E
MOTA	5293	С	SER	Е	118	85.798	66.860	12.377	1.00	17.01	E
MOTA	5294	0	SER	E	118	85.507	67.543	13.354	1.00	16.69	E
ATOM	5295	N	VAL	E	119	85.240	65.688	12.112	1.00	16.58	E
ATOM	5296	CA	VAL	E	119	84.242	65.095	12.985	1.00	16.03	B
MOTA	5297	CB	VAL	E	119	83.040	64.582	12.160	1.00	15.47	E
ATOM	5298	CG1	VAL	E	119	81.918	64.147	13.077		13.75	B
ATOM	5299	CG2	VAL	E	119	82.559	65.686	11.216		10.95	B
ATOM	5300	C	VAL			85.018	63.960	13.638		17.51	E
ATOM	5301	0	VAL			85.238	62.906	13.042		19.30	E
ATOM	5302	N	THR			85.442	64.203	14.871		18.44	E
ATOM	5303	CA	THR			86.265	63.266	15.616		18.41	E
ATOM	5304	СВ	THR			87.562	63.962	16.042		18.11	
ATOM	5305		THR			87.242	65.078	16.887			E
ATOM	5306		THR							17.18	B
ATOM						88.304	64.481	14.835		16.77	E
ATOM	5307	C	THR			85.655	62.656	16.875		20.11	E
	5308	0	THR			84.665	63.148	17.417		21.96	. B
ATOM	5309	N	ASP			86.272	61.566	17.319		19.96	E
ATOM	5310	CA	ASP			85.882	60.864	18.529		21.06	E
ATOM	5311	CB	ASP			86.313	61.686	19.745		25.93	E
ATOM	5312	CG	ASP			87.814	61.765	19.882		30.02	E
ATOM	5313		ASP			88.291	62.524	20.756		34.97	E
ATOM	5314		ASP			88.513	61.063	19.114	1.00	31.15	E
ATOM	5315	C	asp			84.431	60.463	18.709		20.39	B
MOTA	5316	0	ASP	E	121	83.857	60.698	19.766	1.00	22.05	B
MOTA	5317	N	PHB			83.827	59.841	17.708	1.00	19.69	E
MOTA	5318	CA	PHE			82.443	59.429	17.873	1.00	18.28	E
MOTA	5319	СВ	PHE	E	122	81.538	60.108	16.843	1.00	16.99	E
MOTA	5320	CG	PHE	E	122	81.905	59.821	15.417		16.67	E
MOTA	5321		PHE			82.770	60.661	14.725		16.72	E
MOTA	5322		PHE			81.370	58.717	14.756		17.17	E
MOTA	5323		PHE			83.096	60.410	13.384		17.00	E

MOTA	5324	CE2	PHE 1	B	122	81.6	586	58.456	13.419	1.00	16.82	B
ATOM	5325	CZ	PHE 1	8	122	82.5	549	59.305	12.733	1.00	15.81	B
MOTA	5326	С	PHE 1	E	122	82.2	287	57.925	17.774	1.00	18.35	E
ATOM	5327	0	PHE I	E	122	83.3	168	57.231	17.272	1.00	15.90	E
ATOM	5328	N	TYR I			81.3		57.436	18.276		19.49	E
ATOM	5329	CA	TYR I			80.		56.021	18.243		20.92	E
ATOM	5330	СВ	TYR I			81.		55.261	19.374		21.02	В
ATOM		CG	TYR I			81.3		53.762	19.247		20.05	E
	5331											
ATOM	5332		TYR !			80.2		53.103	19.688		21.66	B
MOTA	5333		TYR !			80.		51.726	19.516		21.85	B
ATOM	5334		TYR I			82.3	383	53.009	18.633		20.08	E
ATOM	5335	CE2	TYR I	E	123	82.3	250	51.643	18.455		19.20	B
ATOM	5336	CZ	TYR 1	E,	123	81.3	105	51.002	18.896	1.00	22,24	E
MOTA	5337	OH	TYR :	E	123	80.	970	49.640	18.712	1.00	25.26	E
MOTA	5338	C	TYR :	E	123	79.3	311	55.957	18.440	1.00	21.42	B
MOTA	5339	0	TYR :	E	123	78.	778	56.647	19.309	1.00	23,90	E
ATOM	5340	N	PRO I			78.		55.100	17.676		20.39	E
ATOM	5341	CD	PRO			77.		54.937	17.844		21.24	E
MOTA	5342	CA	PRO 1			79.		54.177	16.65		21.61	B
		СВ	PRO I			77.		53.188	16.500		19.35	B
MOTA	5343							54.056	16.670		19.34	E
ATOM	5344	CG	PRO			76.						
MOTA	5345	C	PRO			79.		54.802	15.329		20.84	B
MOTA	5346	0	PRO 1			79.		56.024	15.184		22.13	B
MOTA	5347	N	ALA :			79.		53.940	14.363		22.61	E
MOTA	5348	CA	ALA :		125	80.		54.341	13.02		25.48	B
MOTA	5349	CB	ALA :	E	125	80.		53.121	12.28	3 1.00	26.06	E
ATOM	5350	C	ALA :	E	125	79.	311	55.058	12.13	7 1.00	27.38	B
MOTA	5351	0	ALA :	E	125	79.	681	55.906	11.33	1.00	29.08	B
ATOM	5352	N	GLN :	E	126	78.	039	54.706	12.26	3 1.00	29.18	E
ATOM	5353	CA	GLN :	E	126	76.	990	55.312	11.45	1.00	29.94	E
ATOM	5354	CB	GLN	E	126	75.		54.737	11.84	3 1.00	33.48	B
ATOM	5355	CG	GLN			75.		53.200	11.84		39.27	E
ATOM	5356	CD CD	GLN			76.		52.537	13.11		41.92	E
			GLN			77.		52.523	13.37		44.02	B
ATOM	5357							51.981	13.91		43.83	E
MOTA	5358		GLN			75.						E
MOTA	5359	C	GLN			76.		56.829	11.62		28.88	
MOTA	5360	0	GLN			76.		57.331	12.71		28.83	8
MOTA	5361	N	ILE			77.		57.558	10.53		27.90	B
ATOM	5362	CA	ILE	E	127	77.	245	59.018	10.59		25.67	R
MOTA	5363	CB	ILE	E	127	78.	611	59.514	11.15	1.00	25.23	В
ATOM	5364	CG2	ILE	E	127	79.	693	59.398	10.08	4 1.00	21.16	E
ATOM	5365	CG1	ILE	E	127	78.	504	60.965	11.61	1.00	22.40	R
ATOM	5366	CD1	ILE	E	127	79.	610	61.376	12.54	5 1.00	25.35	E
MOTA	5367	С	ILE	E	127	76.	985	59.673	9.23	1.00	26.38	E
MOTA	5368	o	ILE				196	59.065	8.18	2 1.00	26.20	В
ATOM	5369	N	LYS				521	60.916	9.25		25.64	В
MOTA	5370	CA	LYS				248	61.635	8.01		29.02	E
ATOM	5371	CB	LYS				754	61.566	7.67		29.97	B
ATOM	5372	CG	LYS		128		408	62.178	6.31		35.17	E
			LYS				175	61.487	5.18		39.63	E
MOTA	5373	CD	LYS								41.20	B
ATOM	5374	CE					936	62.163	3.83		44.74	E
ATOM	5375	NZ	LYS				685	61.492	2.73			
MOTA	5376	C	LYS				683	63.090	8.15		28.40	E
MOTA	5377	0	LYS				203	63.812	9.02		27.15	E
ATOM	5378	N	VAL				600	63.506	7.28		28.99	E
MOTA	5379	CA	VAL				119	64.866	7.30		29.32	E
MOTA	5380	CB	VAL			79.	651	64.860	7.50		30.69	E
ATOM	5381	CG1	VAL	E	129	80.	171	66.282	7.65		27.54	E
MOTA	5382	CG2	VAL	B	129	80.	014	64.012	8.72	_	30.82	E
MOTA	5383	C	VAL	E	129	77.	788	65.574	5.99	2 1.00	30.45	В
ATOM	5384	0	VAL	B	129	78.	042	65.039	4.91	5 1.00	30.36	E
ATOM	5385	N	ARG	В	130	77.	221	66.775	6.09	0 1.00	31.17	E
ATOM	5386	CA	ARG				851	67.562	4.91	4 1.00	32.17	E
MOTA	5387	CB	ARG				330	67.626	4.76		34.73	E
ATOM	5388	CG	ARG				632	66.335	4.40		40.85	E
			ARG				121	66.527	4.51		46.16	E
ATOM	5389	CD	ARG				365	65.456	3.86	_	51.33	E
ATOM	5390	NE							3.95		53.45	E
MOTA	5391	CZ			130		046	65.308		-	54.21	E
ATOM	5392		ARG				327	66.162	4.68		53.97	
MOTA	5393		ARG				444	64.307	3.32			E
ATOM	5394	C			130		359	68.994	5.01		30.88	B
MOTA	5395	0			130		.321	69.590	6.09		30.84	E
MOTA	5396	N			131		831	69.542	3.90		29.14	E
MOTA	5397	CA	TRP	E	131	78.	.291	70.928	3.86	5 1.00	29.57	E

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MOTA	5398	CB	TRP	E 131	79.538	71.086	2.996	1.00 27.97	E
ATOM	5399	CG	TRP	E 131	80.809				E
ATOM	5400	CD:	TRP	E 131	81.342				E
ATOM	5401	CE:	TRP	E 131	82.551			1.00 29.75	
ATOM	5402	CE:	TRP	E 131	80.913	73.209		1.00 30.39	E
ATOM	5403	CD:	TRP	B 131	81.689		3.747	1.00 29.02	E
ATOM	5404	NE:	TRP	B 131	82.738	70.200	4.592	1.00 30.01	E
ATOM	5405	CZ2	TRP	B 131	83.340	72.119	6.095	1.00 28.79	
ATOM	5406	CZ3	TRP	E 131	81.697	73.900	6.027	1.00 31.30	E
ATOM	5407	CH2	TRP	E 131	82.900	73.350	6.509	1.00 31.69	E
ATOM	5408	C	TRP	E 131	77.185	71.817	3.301	1.00 30.08	
ATOM	5409	0	TRP	E 131	76.449	71.413	2.392	1.00 29.15	e e
MOTA	5410	N	PHE	E 132	77.081	73.027	3.842	1.00 29.87	E
ATOM	5411	CA	PHE	B 132	76.078	73.985	3.405	1.00 30.98	E
ATOM	5412	СB	PHE	E 132	74.963	74.094	4.443	1.00 32.09	B
ATOM	5413	CG	PHE	E 132	74.041	72.918	4.461	1.00 33.03	E
MOTA	5414	CD1	PHE	E 132	72.913	72.896	3.650	1.00 35.25	E
ATOM	5415	CD2	PHE	E 132	74.306	71.822	5.273	1.00 33.31	E
ATOM	5416	CE1	PHE	B 132	72.055	71.794	3.646	1.00 35.49	E
ATOM	5417	CE2	PHE	E 132	73.460	70.717	5.279	1.00 35.47	E
ATOM	5418	CZ	PHE	E 132	72.330	70.704	4.461	1.00 35.97	E
ATOM	5419	C	PHB	B 132	76.668	75.364	3.182	1.00 32.06	E
ATOM	5420	0	PHE		77.537	75.812	3.929	1.00 29.15	E
MOTA	5421	N	ARG	E 133	76.186	76.026	2.138	1.00 34.68	B
ATOM	5422	CA		E 133	76.613	77.375	1.809	1.00 37.78	E
ATOM	5423	CB		E 133	77.281	77.420	0.434	1.00 40.14	E
MOTA	5424	CG		E 133	77.755	78.810	0.005	1.00 43.27	B
MOTA	5,425	Э		E 133	78.474	78.742	-1.341	1.00 46.34	E
ATOM	5426	NE		E 133	79.096	80.006	-1.738	1.00 49.86	E
ATOM	5427	CZ		E 133	78.441	81.058	-2.226	1.00 51.63	B
ATOM	5428		ARG :		77.124	81.018	-2.387	1.00 51.33	E
MOTA	5429		ARG :		79.111	82.155	-2.562	1.00 52.46	B
ATOM	5430	C		B 133	75.343	78.204	1.792	1.00 38.70	B
ATOM	5431	0		E 133	74.569	78.154	0.835	1.00 38.81	B
ATOM	5432	N		B 134	75.119	78.940	2.872	1.00 39.37	E
MOTA	5433	CA.		E 134	73.941	79.787	2.984	1.00 42.21	B
ATOM	5434	CB	ASN I		74.040	80.952	1.988	1.00 40.37	E
ATOM	5435	CG	ASN I		75.383	81.667	2.051	1.00 39.50	E
ATOM	5436		ASN I		75.796	82.151	3.104	1.00 35.36	E
ATOM	5437		ASN I		76.071	81.733	0.917	1.00 39.94	E
MOTA	5438	C	ASN I		72.652	79.000	2.734	1.00 43.61	B
MOTA	5439	0	ASN I		71.899	79.306	1.809	1.00 45.62	E
ATOM ATOM	5440	N	ASP I		72.403	77.983	3.550	1.00 45.40	E
ATOM	5441	CA	ASP E		71.189	77.178	3.413	1.00 47.16	E
ATOM	5442 5443	0	ASP I		71.147	76.279	2.173	1.00 48.15	E
ATOM	5444	И	ASP E		70.205	75.504	1.996	1.00 49.25	E
ATOM	5445	CA	GLN E		72.158	76.387	1.316	1.00 48.16	E
ATOM	5446	C	GLN E		72.226	75.561	0.113	1.00 47.50	E
ATOM	5447	0	GLN E		73.254	74.445	0.313	1.00 47.38	E
ATOM	5448	N	GLU E		74.418 72.829	74.711	0.627	1.00 46.25	B
ATOM	5449	CA	GLU E		73.749	73.197	0.139	1.00 47.09	E
ATOM	5450	CB	GLU E		72.992	72.079 70.752	0.308	1.00 47.41	E
ATOM	5451		GLU E		73.921	69.570	0.406 0.653	1.00 47.53	E
MOTA	5452		GLU E		73.210	68.334	1.166	1.00 49.67	E
ATOM	5453		GLU E		73.911	67.336	1.432	1.00 51.28	E
MOTA	5454		GLU E		71.965	68.352	1.306	1.00 52.31 1.00 51.54	E
MOTA	5455		GLU E		74.755	72.016	-0.833	1.00 47.37	E
ATOM	5456		GLU E		74.397	72.163	-2.000	1.00 47.51	B
ATOM	5457		GLU E		76.018	71.809	-0.477	1.00 47.53	e
ATOM	5458	CA	GLU E	138	77.104	71.724	-1.444	1.00 48.48	E
ATOM	5459	CB	GLU E	138	78.266	72.617	-1.011	1.00 49.89	E
MOTA	5460	CG	GLU E	138	77.949	74.096	-0.973	1.00 54.83	E
MOTA	5461	CD	GLU E	138	77.911		-2.354	1.00 57.91	E
MOTA	5462	OE1	GLU E	138	78.953	74.686	-3.044	1.00 59.04	E
MOTA	5463		GLU E		76.846		-2.748	1.00 58.96	E
MOTA	5464		GLU E		77.593		-1.532	1.00 48.42	E
MOTA	5465		GLU E		77.898			1.00 48.62	E
MOTA			THR B		77.665	69.754		1.00 47.87	E
MOTA	5467		THR E		78.135		-2.959	1.00 48.16	E
ATOM	5468		THR E		77.027		-3.556	1.00 49.05	E
MOTA	5469		THR E		76.464		-4.710	1.00 51.25	B
MOTA	5470		THR E		75.938		-2.525	1.00 48.03	E
ATOM	5471	C '	THR E	139	79.339	68.401	-3.895	1.00 46.96	E

MOTA	5472	0		E 139	80.245	67.574	-3.779	1.00 46.46	В
ATOM	5473	N		E 140	79.339	69.346	-4.827	1.00 46.59	E
ATOM	5474	CA		E 140	80.446		-5.761	1.00 45.07	В
ATOM	5475	CB		E 140	79.997		-7.008	1.00 44.64	E
ATOM ATOM	5476 5477	0		B 140	81.518	70.276	-5.019	1.00 43.57	E
ATOM	5478	И		B 140 B 141	81.224	71.293	-4.386	1.00 43.33	B
ATOM	5479	CA		B 141	82.756 83.833	69.805	-5.091	1.00 41.31	B
ATOM	5480	c.		B 141	84.053	70.485 69.854	-4.398	1.00 38.27	E
MOTA	5481	ō		B 141	84.930	70.264	-3.034 -2.272	1.00 36.91 1.00 37.78	E
ATOM	5482	N		3 142	83.245	68.849	-2.722	1.00 37.78	e E
ATOM	5483	CA	VAL I	E 142	83.363	68.164	-1.449	1.00 32.16	E
ATOM	5484	CB	VAL 1		81.978	67.844	-0.847	1.00 31.40	E
ATOM	5485		. VAL I		82.140	66.995	0.407	1.00 28.96	E
ATOM	5486		VAL I		81.245	69.134	-0.516	1.00 33.20	E
ATOM ATOM	5487	C	VAL I		84.140	66.859	-1.576	1.00 31.49	E
ATOM	5488 5489	O N	VAL E		83.862	66.032	-2.450	1.00 31.67	В
ATOM	5490	CA	VAL E		85.118 85.922	66.684 65.473	-0.696	1.00 30.51	E
ATOM	5491	CB	VAL E		87.367	65.731	-0.675 -1.161	1.00 30.35	B
ATOM	5492		VAL E		88.096	64.408	-1.348	1.00 30.33	E
ATOM	5493	CG2	VAL E	143	87.347	66.503	-2.460	1.00 33.96	E
ATOM	5494	C	VAL E		85.966	64.973	0.767	1.00 29.68	E
ATOM	5495	0	VAL E		86.242	65.733	1.695	1.00 29.63	E
ATOM	5496	N	SER E		85.696	63.689	0.946	1.00 28.32	E
ATOM ATOM	5497	CA	SER E		85.703	63.090	2.268	1.00 25.38	E
ATOM	5498 5499	CB OG	SER E		84.295	62.613	2.622	1.00 26.70	E
ATOM	5500	C	SER E		84.300 86.663	61.845 61.916	3.807	1.00 28.37	E
ATOM	5501	ō	SER E		86.824	61.148	2.361 1.412	1.00 24.56 1.00 23.42	E
ATOM	5502	N	THR E		87.320	61.790	3.506	1.00 24.40	e
ATOM	5503	CA	THR E	145	88.218	60.666	3.726	1.00 24.38	E
ATOM	5504	CB	THR E		89.103	60.849	4.983	1.00 24.55	E
ATOM	5505		THR E		88.273	60.815	6.155	1.00 21.59	B
ATOM	5506		THR E		89.858	62.162	4.935	1.00 24.64	E
ATOM ATOM	5507	C	THR E		87.256	59.539	4.055	1.00 23.78	E
ATOM	5508 5509	N O	THR E		86.064	59.766	4.242	1.00 23.97	E
ATOM	5510	CD	PRO E		87.745 88.993	58.300 57.713	4.099	1.00 25.25	E
ATOM	5511	CA	PRO B		86.770	57.264	3.585 4.447	1.00 25.42 1.00 25.00	E
MOTA	5512	CB	PRO E		87.439	55.983	3.951	1.00 26.60	B
ATOM	5513	CG	PRO E	146	88.905	56.293	4.094	1.00 27.24	B
MOTA	5514	C	PRO E		86.597	57.284	5.976	1.00 23.26	E
ATOM	5515	0	PRO B		87.286	58.030	6.672	1.00 21.73	B
ATOM	5516	N	LEU E		85.669	56.492	6.495	1.00 23.85	E
ATOM ATOM	5517 5518	CA CB	TER E		85.476	56.419	7.936	1.00 23.63	E
ATOM	5519	CG	LEU E		84.355	55.428	8.260	1.00 25.11	E
ATOM	5520		TER B		83.976 83.392	55.241 56.530	9.731 10.270	1.00 28.28	E
ATOM	5521		LEU E		82.965	54.116	9.867	1.00 29.44 1.00 28.72	e E
ATOM	5522	C	LEU B		86.812	55.915	8.503	1.00 22.77	B
MOTA	5523	0	LEU E	147	87.366		8.003		E
ATOM	5524	N	ILE E		87.337	56.574	9.530	1.00 21.06	E
ATOM	5525	CA	IFE E		88.614	56.156	10.102	1.00 19.40	E
ATOM ATOM	5526	CB	ILE E		89.588	57.355	10.200	1.00 20.05	E
ATOM	5527 5528		ILE E		90.903	56.922	10.835	1.00 19.93	E
ATOM	5529		ILE E		89.854 90.594	57.918 59.225	8.803 8.821	1.00 17.58	E
ATOM	5530	c	ILE E		88.449	55.534	11.489	1.00 20.23 1.00 17.19	E
ATOM	5531	0	ILB B		87.820	56.118	12.360	1.00 15.81	E
MOTA	5532	N	ARG E		89.015	54.344	11.677	1.00 15.23	E
ATOM	5533	CA	ARG E		88.948	53.638	12.956	1.00 16.42	E
MOTA	5534	CB	ARG E		88.906	52.128	12.724	1.00 20.12	B
ATOM	5535	CG	ARG E		88.903	51.289	14.000	1.00 21.32	E
ATOM	5536 5537	CD	ARG E		88.963	49.802	13.649	1.00 22.44	E
ATOM ATOM	5537 5538	ne Cz	ARG E		87.825 86.633	49.382	12.830	1.00 22.55	E
ATOM	5539		ARG E	149 .	86.623 85.650	49.084 48.718	13.313	1.00 22.89	E
MOTA	5540		ARG E		86.398	49.139	12.490 14.619	1.00 24.25 1.00 23.36	E
MOTA	5541	C	ARG E		90.174	53.983	13.786	1.00 23.36	e
ATOM	5542	0	ARG E		91.305	53.734	13.363	1.00 16.45	E
MOTA	5543	N	ASN E		89.953	54.558	14.963	1.00 15.72	B
ATOM	5544	CA	ASN E		91.061	54.948	15.825	1.00 15.93	E
ATOM	5545	CB	asn e	150	90.662	56.125	16.740	1.00 13.37	E

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MOTA	5546	CG	asn e	150	90.278	57.383	15.955	1.00 15.55	E
MOTA	5547	OD1	ASN B	150	90.922	57.739	14.955	1.00 14.20	E
MOTA	5548		ASN E		89.233	58.068	16.414	1.00 15.61	E
ATOM	5549	C	ASN E		91.576	53.786	16.670	1.00 16.79	E
							17.180	1.00 18.80	B _
MOTA	5550	0	ASN E		92.694	53.838			
MOTA	5551	N	GLY E		90.764	52.745	16.813	1.00 16.63	E
MOTA	5552	CA	GLY E	151	91.164	51.587	17.593	1.00 18.68	B
ATOM	5553	C	GLY E	151	90.879	51.684	19.080	1.00 20.19	E
ATOM	5554	ō	GLY E		91.087	50.725	19.818	1.00 21.39	E
					90,409	52.836	19.539	1.00 19.57	E
MOTA	5555	N	ASP E						
ATOM	5556	CA	ASP E	152	90.108	52.986	20.954	1.00 19.09	E
ATOM	5557	CB	ASP E	152	90.865	54.177	21.531	1.00 18.53	E
MOTA	5558	CG	ASP E	152	90.498	55.481	20.856	1.00 21.27	E
ATOM	5559		ASP E	152	89.736	55.453	19.864	1.00 20.11	E
					90.984	56.531	21.321	1.00 22.57	E
MOTA	5560		ASP E						E
ATOM	5561	С	ASP E		88.605	53.156	21.182	1.00 19.23	
MOTA	5562	0	ASP E	152	88.177	53.840	22.113	1.00 17.78	B
ATOM	5563	N	TRP E	153	87.816	52.522	20.318	1.00 18.88	E
ATOM	5564	CA	TRP B	153	86.356	52.566	20.391	1.00 18.61	E
ATOM	5565	СВ	TRP E		B5.862	52.162	21.788	1.00 17.06	E
					86.084	50.690	22.085	1.00 17.90	E
MOTA	5566	CG	TRP E						E
MOTA	5567	CD2	TRP E		85.165	49.612	21.830	1.00 18.84	
ATOM	5568	CE2	TRP E	153	85.804	48.414	22.222	1.00 16.88	E
ATOM	5569	CE3	TRP E	153	83.862	49.544	21.308	1.00 18.29	B
ATOM	5570	CD1	TRP E	153	87.209	50.114	22.604	1.00 16.70	B
			TRP E		87.049	48.747	22.688	1.00 17.49	B
ATOM	5571							1.00 16.54	E
MOTA	5572		TRP E		85.189	47.164	22.109		
MOTA	5573	CZ3	TRP E	153	83.250	48.303	21.196	1.00 17.19	B
MOTA	5574	CH2	TRP E	153	83.917	47.129	21.597	1.00 17.24	B
ATOM	5575	C	TRP B	153	85.732	53.887	19.975	1.00 18.97	R
	5576	ŏ	TRP E		84.696	54.300	20.508	1.00 18.70	E
MOTA						54.546	19.016	1.00 19.20	E
MOTA	5577	N	THR E		86.378				
MOTA	5578	CA	THR E		85.876	55.794	18.444	1.00 19.92	E
ATOM	5579	CB	THR E	154	86.442	57.072	19.129	1.00 21.42	E
MOTA	5580	OG1	THR E	154	87.865	57.129	18.958	1.00 19.26	E
MOTA	5581	CG2	THR E	154	86,085	57.096	20.599	1.00 22.17	E
		C	THR E		86.314	55.835	16.992	1.00 18.66	E
MOTA	5582							1.00 19.45	E
MOTA	5583	0	THR E		87.270	55.156	16.603		
MOTA	5584	N	PHE E	155	85.609	56.626	16.193	1.00 18.54	E
ATOM	5585	CA	PHE E	155	85.940	56.784	14.779	1.00 19.04	E
MOTA	5586	CB	PHE E	155	84.821	56.252	13.882	1.00 20.71	E
ATOM	5587	CG	PHE E	155	84.524	54.794	14.060	1.00 23.03	B
			. PHE E		83.492	54.375	14.898	1.00 23.94	Ē
MOTA	5588						13.365	1.00 23.32	E
MOTA	5589		PHE E		85.255	53.837			
MOTA	5590	CE1	. PHE E	155	83.189	53.017	15.037	1.00 23.82	E
MOTA	5591	CE2	PHE F	155	84.962	52.476	13.497	1.00 24.46	E
MOTA	5592	CZ	PHE E	1.55	83.930	52.068	14.333	1.00 24.51	B
ATOM	5593	C	PHE F	155	86.109	58.265	14.459	1.00 19.30	B
	5594		PHE E		85.791	59.134	15.275	1.00 19.12	E
MOTA		0					13.265	1.00 17.46	B
MOTA	5595	N	GTM E		86.613	58.550			
MOTA	5596	CA	GLN F	3 156	86.748	59.924	12.824	1.00 17.87	B
ATOM	5597	CB	GLN I	3 156	88.081	60.546	13.264	1.00 19.74	E
ATOM	5598	CG	GLN I	3 156	89.330	59.948	12.640	1.00 19.80	B
MOTA	5599	CD	GLN I	3 156	90.551	60.785	12.950	1.00 21.46	E
ATOM	5600		L GLN I		90.660	61.92B	12.503	1.00 21.30	E
					91.469	60.230	13.734	1.00 21.38	E
ATOM	5601	NE						1.00 17.47	B
MOTA	5602	C		E 156	86.629	59.989	11.316		
ATOM	5603	0	GLN I	E 156	86.856	58.999	10.616	1.00 17.25	E
MOTA	5604	N	ILE 1	<b>5 157</b>	86.252	61.159	10.823	1.00 17.46	E
MOTA	5605	CA	ILE !	E 157	86.128	61.363	9.397	1.00 18.92	E
ATOM	5606	CB		E 157	84.746	60.922	8.898	1.00 19.57	E
	5607		2 ILE 1		83.659	61.774	9.545	1.00 15.09	E
ATOM								1.00 21.06	E
MOTA	5608		L ILE		84.704	60.994	7.369		
MOTA	5609	CD:	l ILE		83.541	60.218	6.756	1.00 22.57	E
MOTA	5610	C	ILE :	E 157	86.349	62.837	9.083	1.00 20.28	B
MOTA	5611	0	ILE	B 157	85.887	63.712	9.808	1.00 20.70	E
MOTA	5612	N		E 158	87.094	63.104	8.019	1.00 21.79	E
ATOM	5613	CA		E 158	87.363	64.470	7.601	1.00 23.40	B
					88.869	64.706	7.466	1.00 25.42	B
MOTA	5614			E 158					E
MOTA	5615			E 158	89.621		8.731	1.00 29.38	
ATOM	5616		1 LEU		89.384	64.154	9.864	1.00 27.98	B
ATOM	5617	CD	2 LEU	E 158	91.118	65.263	8.412	1.00 30.79	B
ATOM	5618			E 158	86.664	64.738	6.271	1.00 23.62	E
ATOM	5619			E 158	86.938		5.264	1.00 22.86	E
ALUM.		•							

				05 747	CE 702	6.290	1.00 22.98	В
ATOM	5620	N	VAL E 159	85.747	65.702		1.00 22.30	E
ATOM	5621	CA	VAL E 159	84.990	66.087	5.112	1.00 20.53	E
MOTA	5622	CB	VAL E 159	83.476	66.104	5.417		
MOTA	5623		VAL E 159	82.684	66.407	4.149	1.00 14.20	E
MOTA	5624	CG2	VAL E 159	83.058	64.756	6.002	1.00 15.86	8
MOTA	5625	C	VAL E 159	85.468	67.469	4.710	1.00 22.21	E
MOTA	5626	0	VAL B 159	85.253	68.444	5.423	1.00 22.87	E
ATOM	5627	N	MET E 160	86.116	67.539	3.555	1.00 25.37	E
ATOM	5628	CA	MET E 160	86.681	68.779	3.049	1.00 27.07	E
MOTA	5629	СВ	MET E 160	88.088	68.494	2.533	1.00 29.57	E
ATOM	5630	CG	MET B 160	88.996	67.954	3.633	1.00 35.17	E
ATOM	5631	SD	MET E 160	90.519	67.185	3.065	1.00 41.54	E
	5632	CE	MET E 160	90.011	65.462	2.985	1.00 40.10	E
MOTA			MET E 160	85.848		1.979	1.00 28.93	E
ATOM	5633	C		85.191	68.817	1.162	1.00 28.47	E
MOTA	5634	0	MET E 160		70.793	1.997	1.00 29.41	E
MOTA	5635	N	LEU E 161	85.875			1.00 31.54	B
ATOM	5636	CA	LEU E 161	85.123	71.574	1.031		E
MOTA	5637	CB	LEU E 161	83.931	72.258	1.708	1.00 30.26	
MOTA	5638	CG	LEU E 161	83.183	73.297	0.860	1.00 30.70	E
MOTA	5639	CD1	LEU E 161	82.515	72.618	-0.332	1.00 29.72	E
ATOM	5640	CD2	LBU E 161	82.145	74.020	1.728	1.00 31.55	E
MOTA	5641	C	LEU E 161	85.990	72.625	0.363	1.00 32.10	B
MOTA	5642	0	LEU E 161	86.575	73.473	1.029	1.00 32.90	B
ATOM	5643	N	GLU E 162	86.063	72.549	-0.960	1.00 35.11	E
MOTA	5644	CA	GLU E 162	86.820	73.491	-1.771	1.00 38.40	E
ATOM	5645	СВ	GLU E 162	87.191	72.838	-3.105	1.00 42.17	B
		CG	GLU B 162	87.783	73.776	-4.148	1.00 48.21	B
MOTA	5646			89.099	74.381	-3.711	1.00 52.47	E
ATOM	5647	CD	GLU R 162		73.611	-3.327	1.00 54.02	B
MOTA	5648		GLU E 162	90.006			1.00 56.21	E
ATOM	5649	OE2		89.228	75.627	-3.759		E
ATOM	5650	С	GLU E 162	85.892	74.673	-2.008	1.00 39.06	
MOTA	5651	0	GLU E 162	84.750	74.490	-2.422	1.00 39.27	E
MOTA	5652	N	MET E 163	86.369	75.884	-1.747	1.00 40.73	E
ATOM	5653	CA	MET E 163	85.520	77.049	-1.938	1.00 43.18	E
MOTA	5654	CB	MET E 163	84.546	77.171	-0.761	1.00 45.15	E
ATOM	5655	CG	MET B 163	85.155	76.900	0.612	1.00 47.55	E
ATOM	5656	SD	MET E 163	86.318	78.152	1.185	1.00 52.18	B
MOTA	5657	CE	MET B 163	85.186	79.345	1.941	1.00 50.37	E
MOTA	5658	c	MET E 163	86.245	78.371	-2.151	1.00 43.77	E
	5659	ō	MET E 163	87.458	78.477	-1.953	1.00 41.87	E
ATOM			THR E 164	85.474	79.371	-2.571	1.00 45.83	E
MOTA	5660	N			80.714	-2.827	1.00 49.20	E
ATOM	5661	CA	THR E 164	85.981	81.177	-4.241	1.00 50.11	E
MOTA	5662	CB	THR E 164	85.585			1.00 49.28	E
ATOM	5663		THR E 164	86.036	80.208	-5.199		E
ATOM	5664	CG2		86.204	82.535	-4.559	1.00 50.19	E
ATOM	5665	C	THR E 164	85.371	81.652	-1.785	1.00 51.14	E
ATOM	5666	0	THR B 164	84.169	81.916	-1.802	1.00 50.64	
MOTA	5667	N	PRO E 165	86.198	82.170	-0.864	1.00 53.75	E
MOTA	5668	CD	PRO B 165	87.667	82.057	-0.818	1.00 54.65	B
ATOM	5669	CA	PRO E 165	85.719	83.072	0.185	1.00 56.16	E
ATOM	5670	CB	PRO E 165	86.965	83.299	1.036	1.00 55.47	E
ATOM	5671	CG	PRO E 165	88.057	83.262	0.019	1.00 55.93	E
ATOM	5672	C	PRO E 165	85.098	84.381	-0.291	1.00 58.83	E
MOTA	5673	0	PRO E 165	85.673	85.100	-1.112	1.00 58.35	E
ATOM	5674	N	GLN E 166	83.912	84.666	0.239	1.00 61.77	E
ATOM	5675	CA	<b>GLN E 166</b>	83.173	85.885	-0.065	1.00 63.96	E
MOTA	5676	CB	GLN E 166	82.103	85.616	-1.123	1.00 64.28	E
ATOM	5677	CG	GLN E 166	82.662	85.236	-2.481	1.00 66.42	E
		CD CD	GLN E 166	81.643	85.392	-3.596	1.00 67.38	E
ATOM	5678			81.937	85,124	-4.761	1.00 68.28	. E
MOTA	5679		1 GLN E 166			-3.244	1.00 66.50	E
ATOM	5680		2 GLN B 166	80.437	85.832	1.223	1.00 65.40	E
ATOM	5681	C	GLN E 166	82.521	86.396			E
MOTA	5682	0	GLN E 166	81.974	85.614	2.007		E
ATOM	5683	N	ARG E 167	82.589	87.707	1.444	1.00 65.80	
MOTA	5684	CA		82.017		2.647		E
MOTA	5685	CB	ARG E 167	82.353	89.795	2.706		E
ATOM	5686	CG	ARG E 167	82.221	90.423	4.095		E
ATOM	5687		ARG E 167	83.216	89.813	5.085		E
MOTA	5688		ARG E 167	83.244	90.532	6.359		E
ATOM	5689			84.012		7.394	1.00 75.48	E
ATOM	5690		1 ARG E 167	84.824				E
ATOM	5691		2 ARG E 167	83.968		8.509		E
ATOM	5692		ARG E 167	80.504				E
ATOM			ARG E 167	79.816		1.672		B
WI OM	5693	J	MAG E TO	,,,,,,,				

MOTA	5694	N	<b>GLY E 168</b>	79.991	87.751	3.860	1.00 61.88	e
MOTA	5695	CA	GLY E 168	78.567	87.519	4.004	1.00 58.78	B
MOTA	5696	c	GLY E 168	78.243	86.036	3.959	1.00 57.24	E
								<b>B</b>
MOTA	5697	0	GTA E 168	77.262	85.594	4.558	1.00 57.26	
MOTA	5698	N	ASP E 169	79.066	85.263	3.249	1.00 54.67	E
MOTA	5699	CA	ASP E 169	78.849	83.823	3.140	1.00 52.07	E
MOTA	5700	CB	ASP B 169	79.799	83.186	2.116	1.00 52.03	E
MOTA	5701	CG	ASP E 169	79.329	83.359	0.683	1.00 52.57	E
			ASP E 169	78.105	83.453	0.457	1.00 51.86	E
ATOM	5702							
MOTA	5703	OD2	ASP E 169	80.188	83.376	-0.223	1.00 52.34	E
MOTA	5704	C	ASP E 169	79.027	83.096	4.463	1.00 49.54	E
MOTA	5705	0	ASP E 169	79.993	83.322	5.196	1.00 49.84	E
MOTA	5706	N	VAL E 170	78.082	82.214	4.758	1.00 46.54	E
ATOM	5707	CA	VAL E 170	78.136	81.418	5.970	1.00 43.15	B
						6.871	1.00 42.70	E
MOTA	5708	CB	VAL E 170	76.903	81.669			
MOTA	5709		VAL E 170	76.997	80.819	8.138	1.00 41.36	E
ATOM	5710	CG2	VAL E 170	76.814	83.146	7.227	1.00 41.14	E
MOTA	5711	C	VAL E 170	78.172	79.948	5.555	1.00 41.66	e
MOTA	5712	0	VAL E 170	77.216	79.432	4.972	1.00 40.25	E
ATOM	5713	N	TYR E 171	79.289	79.287	5.833	1.00 39.16	E
						5.502	1.00 38.16	E
MOTA	5714	CA	TYR E 171	79.438	77.877			
MOTA	5715	CB	TYR E 171	80.836	77.617	4.953	1.00 38.66	E
MOTA	5716	CG	TYR E 171	81.035	78.237	3.598	1.00 38.98	E
ATOM	5717	CD1	TYR E 171	80.740	77.522	2.440	1.00 38.79	E
ATOM	5718	CE1	TYR E 171	80.852	78.105	1.186	1.00 40.42	E
	5719		TYR E 171	81.451	79.561	3.471	1.00 38.62	E
MOTA						2.219	1.00 40.32	E
MOTA	5720	CE2		81.565	80.160			
ATOM	5721	$\mathbf{cz}$	TYR B 171	81.262	79.424	1.079	1.00 41.26	E
MOTA	5722	OH	TYR E 171	81.350	80.004	-0.166	1.00 42.98	B
MOTA	5723	C	TYR E 171	79.206	77.076	6.764	1.00 37.15	B
ATOM	5724	0	TYR E 171	79.755	77.398	7.813	1.00 37.94	E
	5725	N	THR E 172	78.384	76.037	6.672	1,00 35.12	B
ATOM					75.229	7.842	1.00 34.42	E
MOTA	5726	CA	THR E 172	78.091				
MOTA	5727	CB	THR E 172	76.654	75.496	8.367	1.00 35.21	E
MOTA	5728	OGI	THR E 172	76.184	74.351	9.094	1.00 35.96	B
ATOM	5729	CG2	THR E 172	75.706	75.790	7.226	1.00 38.35	E
MOTA	5730	C	THR E 172	78.263	73.734	7.638	1.00 32.90	B
MOTA	5731	ō	THR E 172	77.875	73.188	6.604	1.00 31.57	E
					73.090	8.643	1.00 30.59	B
MOTA	5732	N	CYS E 173	78.858				E
MOTA	5733	CA	CYS E 173	79.078	71.646	8.640	1.00 29.35	
MOTA	5734	С	CYS E 173	77.923	71.058	9.454	1.00 29.72	E
ATOM	5735	0	CYS E 173	77.771	71.337	10.645	1.00 28.89	E
MOTA	5736	CB	CYS E 173	80.424	71.299	9.287	1.00 27.53	E
ATOM	5737	SG	CYS E 173	80.875	69.541	9.133	1.00 27.81	E
			HIS E 174	77.109	70.251	8.788	1.00 28.95	E
MOTA	5738	N				9.381	1.00 28.54	E
MOTA	5739	CA	HIS E 174	75.925	69.642			
MOTA	5740	CB	HIS E 174	74.770	69.881	8.399	1.00 29.66	E
ATOM	5741	CG	HIS E 174	73.457	69.311	8.823	1.00 30.98	E
ATOM	5742	CD2	HIS E 174	72.367	69.899	9.369	1.00 31.91	E
MOTA	5743	ND:	L HIS E 174	73.124	67.988	8.630	1.00 31.68	E
ATOM	5744		HIS E 174	71.883	67.785	9.034	1.00 33.26	B
				71.401	68.929	9.487	1.00 34.66	E
MOTA	5745		2 HIS E 174			9.650	1.00 27.83	E
MOTA	5746	C	HIS E 174	76.173	68.151			
ATOM	5747	0	HIS E 174	76.438	67.375	8.728	1.00 27.35	B
ATOM	5748	N	VAL E 175	76.085	67.753	10.917	1.00 26.27	E
ATOM	5749	CA	VAL E 175	76.349	66.365	11.284	1.00 26.34	E
ATOM	5750	CB	VAL E 175	77.584	66.281	12.215	1.00 23.90	E
ATOM	5751		L VAL B 175	77.807	64.850	12.663	1.00 19.67	E
			2 VAL E 175	78.818	66.813	11.491	1.00 19.93	B
ATOM	5752			75.199		11.938	1.00 27.67	E
MOTA	5753	C	VAL E 175		65.603			E
ATOM	5754	0	VAL E 175	74.587	66.064	12.904	1.00 26.77	
MOTA	5755	N	GLU E 176	74.917	64.423	11.399	1,00 29.83	ß
MOTA	5756	CA	GLU E 176	73.864	63.564	11.929	1.00 32.99	E
ATOM	5757		GLU E 176	72.842	63.231	10.839	1.00 34.86	E
ATOM	5758		GLU E 176	72.076	64.441	10.319	1.00 40.13	E
				71.204	64.107	9.124	1.00 44.38	E
MOTA	5759		GLU E 176				1.00 46.31	E
ATOM	5760			70.292	63.265	9.269		
ATOM	5761	OE	2 GLU E 176	71.433	64.682	8.037	1.00 47.49	E
MOTA	5762	С	GLU E 176	74.526	62.289	12.445	1.00 32.24	B
ATOM	5763		GLU E 176	75.296	61,646	11.734	1.00 32.81	E
ATOM	5764		HIS E 177	74.220	61.934	13.686	1.00 31.66	E
				74.803	60.761	14.311	1.00 30.50	E
MOTA	5765						1.00 29.59	E
MOTA	5766			76.147	61.161	14.927		E
ATOM	5767	CG	HIS E 177	76.871	60.034	15.582	1.00 28.23	2

MOTA	5768	CD2	HIS E 17'	77.752	59.134	15.086	1.00 28.22	B
MOTA	5769	ND1	HIS E 17	76.679	59.698	16.903	1.00 27.71	E
ATOM	5770		HIS E 17		58.636	17.194	1.00 29.83	E
					58.274	16.108	1.00 29.78	B
MOTA	5771		HIS E 17					
MOTA	5772	C	HIS E 17		60.195	15.373	1.00 30.09	E
MOTA	5773	0	HIS E 17	73.189	60.942	16.083	1.00 29.91	E
MOTA	5774	N	PRO E 17	73.781	58.862	15.496	1.00 31.45	B
ATOM	5775	CD	PRO E 17	74.485	57.842	14.697	1.00 31.00	E
	5776	CA	PRO E 17		58.226	16.481	1.00 31.44	E
MOTA								
MOTA	5777	CB	PRO E 17		56.779	16.467	1.00 30.89	B
ATOM	5778	CG	PRO E 17	3 73.704	56.578	15.028	1.00 31.16	E
ATOM	5779	С	PRO E 17	72.896	58.826	17.893	1.00 31.78	B
ATOM	5780	0	PRO E 17		58.727	18.611	1.00 32.84	B
	5781	N	SER E 17		59.448	18.292	1.00 30.31	B
ATOM								E
MOTA	5782	CA	SER E 17		60.039	19.624	1.00 30.84	
MOTA	5783	CB	SER E 17	75.552	60.155	20.038	1.00 29.11	B
MOTA	5784	OG	SER E 17	76.240	61.049	19.176	1.00 24.79	B
ATOM	5785	C	SER E 17	73,452	61.424	19.717	1.00 32.75	E
MOTA	5786	ō	SER E 17		61.982	20.804	1.00 32.78	B
						18.583	1.00 35.18	B
MOTA	5787	N	LEU E 18		61.981			
MOTA	5788	CA	TER E 18		63.317	18.578	1.00 37.31	B
MOTA	5789	CB	LEU E 18	73.098	64.132	17.448	1.00 35.77	E
ATOM	5790	CG	LEU E 18	74.610	64.337	17.528	1.00 36.46	B
ATOM	5791		LEU E 18		65.018	16.259	1.00 35.16	E
					65.167	18.752	1.00 34.58	B
MOTA	5792		LEU E 18					
ATOM	5793	C	LEU E 18		63.405	18.463	1.00 40.35	B
ATOM	5794	0	LEU E 18	70.386	63.003	17.456	1.00 40.67	B
MOTA	5795	N	GLN E 18	1 70.338	63.943	19.503	1.00 42.97	B
ATOM	5796	CA	GLN E 18		64.141	19.504	1.00 45.09	E
					64.877	20.776	1.00 46.73	B
MOTA	5797	CB	GLN E 18					
MOTA	5798	CG	GLN E 18		65.931	21.235	1.00 49.84	B
MOTA	5799	CD	GLN E 18	1 68.898	66.904	22.256	1.00 52.17	E
ATOM	5800	OE1	GLN E 18	1 68.074	67.760	21.920	1.00 52.91	E
ATOM	5801	NE2	GLN E 18	1 69.329	66.774	23.510	1.00 51.73	E
		c	GLN E 18		65.002	18.277	1,00 45.26	B
MOTA	5802						1.00 46.25	E
ATOM	5803	0	GLN E 18		64.752	17.530		
ATOM	5804	N	SER E 18	2 69.448	66.013	18.078	1.00 44.33	B
MOTA	5805	CA	SER E 18	2 69.335	66.923	16.943	1.00 42.52	E
ATOM	5806	CB	SER E 18	2 68.819	68.291	17.401	1.00 43.41	E
MOTA	5807	OG	SER E 18		68.853	18.396	1.00 43.07	E
					67.068	16.337	1.00 41.70	E
MOTA	5808	C	SER E 18					
ATOM	5809	0	SER E 18		66.955	17.040	1.00 39.94	E
ATOM	5810	N	PRO E 18	3 70.805	67.330	15.023	1.00 41.57	E
MOTA	5811	CD	PRO E 18	3 69.680	67.554	14.098	1.00 41.72	E
ATOM	5812	CA	PRO E 18	3 72.087	67.485	14.326	1.00 40.68	E
		СВ	PRO E 18		67.638	12.865	1.00 40.95	E
ATOM	5813			-		12.965	1.00 42.76	E
MOTA	5814	CG	PRO E 18		68.309			
ATOM	5815	С	PRO E 18	3 72.988	68.628	14.790	1.00 38.81	E
ATOM	5816	0	PRO E 18	3 72.520	69.709	15.142	1.00 39.64	B
MOTA	5817	N	ILE E 18	4 74.291	68.370	14.785	1.00 37.31	E
ATOM	5818	CA	ILE E 18	4 75.270	69.368	15.177	1.00 34.30	E
		СВ	ILE E 18		68.728	15.699	1.00 33.43	E
ATOM	5819						1.00 32.87	E
MOTA	5820		ILE E 18		69.779	15.766		E
MOTA	5821		ILE E 18		68.112	17.076	1.00 33.53	
MOTA	5822	CD1	ILE E 18	4 77.530	67.339	17.604	1.00 33.29	E
MOTA	5823	С	ILE E 18	4 75.625	70.216	13.974	1.00 33.68	E
MOTA	5824	0	ILE E 18	4 75.851	69.704	12.882	1.00 33.87	E
		N	THR E 18		71.521	14.181	1.00 34.19	E
MOTA	5825						1.00 33.39	E
MOTA	5826	CA	THR E 18		72.431	13.111		
MOTA	5827	CB	THR E 18	5 74.792	73.230	12.637	1.00 33.77	E
ATOM	5828	OG1	THR E 18	5 74.211	73.918	13.751	1.00 33.46	E
ATOM	5829		THRE 18		72.297	12.016	1.00 33.35	B
ATOM	5830	c	THRE 18		73.396	13.590	1.00 33.01	E
					73.966	14.679	1.00 33.25	E
MOTA	5831	0	THRE 18					
MOTA	5832	N	VAL E 18		73.552	12.770	1.00 32.85	E
MOTA	5833	CA	VAL E 18	6 79.197	74.453	13.067	1.00 32.84	E
ATOM	5834	CB	VAL E 18	6 80.503	73.684	13.300	1.00 31.58	E
ATOM	5835		VAL E 1			13.611	1.00 30.07	B
MOTA	5836		VAL E 1			14.441	1.00 30.84	B
						11.836	1.00 34.14	B
ATOM	5837	C	VAL E 1		75.317			
ATOM	5838	0	VAL E 1			10.719	1.00 33.50	E
MOTA	5839	N	GLU E 1	37 79.329		12.029	1,00 38.05	B
ATOM	5840	CA	GLU E 1	79.453	77.522	10.898	1.00 40.60	B
MOTA	5841	СВ	GLU E 1			10.934	1.00 43.36	B

ATOM	5842	CG	GLU !	R	187	78.426	79.531	12.121	1.00 47.46	В
ATOM	5843	CD CD	GLU I			77.657	80.822	11.886	1.00 51.49	E
ATOM	5844	OE1	GLU :	E	187	76.452	80.752	11.551	1.00 52.89	B
MOTA	5845	OE2	GLU :	E	187	78.262	81.908	12.039	1.00 53.48	E
ATOM	5846	C	GLU :	E	187	80.819	78.182	10.877	1.00 40.49	E
ATOM	5847	0	GLU :	E	187	81.496	78.285	11.901	1.00 40.26	E
ATOM	5848	N	TRP :	E	188	81.221	78.610	9.688	1.00 41.52	E
MOTA	5849	CA	TRP :	E	188	82.492	79.284	9.488	1.00 43.59	E
MOTA	5850	CB	TRP	Е	188	83.498	78.337	8.834	1.00 41.24	E
MOTA	5851	CG	TRP	E	188	84.852	78.942	8.675	1.00 41.34	E
MOTA	5852		TRP			85.327	79.672	7.543	1.00 40.23	E
ATOM	5853	CE2	TRP		188	86.642	80.090	7.838	1.00 41.87	E
MOTA	5854	CE3	TRP			84.768	80.015	6.305	1.00 40.90	E
ATOM	5855		TRP		188	85.867	78.945	9.588	1.00 41.88	E
ATOM	5856	NE1	TRP			86.947 87.411	79.632 80.835	9.093 6.938	1.00 41.99 1.00 42.93	E
MOTA MOTA	5857 5858	CZ2	TRP			85.531	80.757	5.408	1.00 42.58	E
ATOM	5859		TRP			86.839	81.159	5.731	1.00 43.65	B
ATOM	5860	C	TRP		188	82.198	80.467	8.566	1.00 46.04	E
ATOM	5861	ō	TRP			81.335	80.374	7.688	1.00 45.30	B
ATOM	5862	N	ARG			82.899	81.579	8.765	1.00 50.26	E
MOTA	5863	CA	ARG			82.673	82.761	7.936	1.00 54.31	E
ATOM	5864	CB	ARG	B	189	81.980	83.855	8.755	1.00 56.19	E
ATOM	5865	CG	ARG	E	189	82.820	84.460	9.880	1.00 59.58	B
ATOM	5866	CD	ARG	E	189	83.030	83.499	11.045	1.00 63.51	E
ATOM	5867	NB	ARG	E	189	83.580	84.180	12.218	1.00 66.73	E
ATOM	5868	CZ	ARG			84.771	84.771	12.255	1.00 68.44	E
ATOM	5869		ARG			85.553	84.766	11.183	1.00 69.41	E
MOTA	5870		ARG			85.178	85.378	13.363	1.00 70.13	E
MOTA	5871	C	ARG		189	83.950	83.322	7.313	1.00 55.74	E
MOTA	5872	0	ARG			85.043	83.182	7.866	1.00 56.16	e E
ATOM	5873	N	ALA			83.796	83.962	6.156 5.435	1.00 58.53	E
MOTA	5874	CA	ALA ALA			84.920 84.550	84.557 84.734	3.964	1.00 59.97	E
ATOM	5875 5876	CB C	ALA			85.335	85.905	6.036	1.00 61.01	E
ATOM ATOM	5877	0	ALA			84.654	86.378	6.971	1.00 62.25	E
ATOM	5878		ALA		190	86.338	86.479	5.558	1.00 61.85	E
MOTA	5879	C	LEU		1	78.718	38.094	33.366	1.00 32.03	F
ATOM	5880	ō	LEU		1	79.818	38.571	33.658	1.00 30.77	F
ATOM	5881	N	LEU		1	76.219	38.100	33.307	1.00 33.21	F
MOTA	5882	CA	LEU		ı	77,432	38.678	33.953	1.00 32.59	F
ATOM	5883	N	GLN	F	2	78.578	37.069	32.531	1.00 30.39	F
ATOM	5884	CA	GLN	F	2	79.744	36.436	31.936	1.00 28.84	F
MOTA	5885	С	GLN	F	2	79.609	36.081	30.462	1.00 27.93	F
MOTA	5886	0	GLN		2	78.741	35.308	30.067	1.00 27.68	F
ATOM	5887	N	PRO		3	80.463	36.663	29.619	1.00 28.02	F
MOTA	5888	CD	PRO		3	81.461	37.720	29.856	1.00 28.68	P P
ATOM	5889	CA	PRO		3	80.370	36.332 37.298	28.198 27.552	1.00 27.76 1.00 28.01	F
MOTA	5890	CB	PRO		3 3	81.363 82.353	37.575	28.660	1.00 28.41	F
ATOM	5891 5892	CG C	PRO		3	80.774	34.872	28.030	1.00 27.24	F
ATOM ATOM	5893	Ö	PRO		3	81.698	34.406	28.698	1.00 27.18	F
ATOM	5894	И	PHE		4	80.082	34.144	27.159	1.00 25.22	F
ATOM	5895	CA	PHE		4	80.409	32.738	26.943	1.00 24.75	F
ATOM	5896	CB	PHE		4	79.135	31.905	26.849	1.00 25.85	F
ATOM	5897	CG	PHE		4	79.272	30.539	27.446	1.00 31.58	F
MOTA	5898	CD1	PHE	F	4	79.435	30.384	28.823	1.00 33.24	F
ATOM	5899	CD2	PHE	F	4	79.241	29.404	26.639	1.00 32.15	F
MOTA	5900		PHE			79.561		29.386	1.00 33.28	F
MOTA	5901		PHE			79.364		27.187	1.00 33.29	F
MOTA	5902	CZ	PHE			79.524	27.989	28.565	1.00 34.18	F
ATOM	5903	C	PHE			81.227		25.664	1.00 22.43	F F
MOTA	5904	0	PHE			80.759		24.586	1.00 24.59	
ATOM	5905	И	PRO			82.460 83.191		25.771 27.029	1.00 22.79 1.00 21.18	F F
MOTA	5906	CD	PRO			83.349		24.618	1.00 21.18	F
MOTA MOTA	5907 5908	CA CB	PRO PRO			84.715		25.218	1.00 20.19	¥
ATOM	5908	CG	PRO			84.587		26.544	1.00 20.99	F
MOTA	5910	G	PRO			83.291		23.949	1.00 20.28	F
ATOM	5911	ŏ	PRO			82.796		24.521	1.00 19.48	F
ATOM	5912	N	GLN			83.818			1.00 21.24	F
MOTA	5913	CA	GLN		6	83.848			1.00 19.98	F
ATOM	5914	СВ	GLN			83.665		20.484	1.00 18.71	F
ATOM	5915	CG	GLN	F	, 6	82.312	30.010	20.048	1.00 18.35	F

MOTA	5916	CD	GLN	₽	6	B2.255	30.247	18.537	1.00 22.29	F
ATOM	5917		GLN		6	82.612	29.368	17.740	1.00 21.53	F
ATOM	5918		GLN		6	81.802	31.429	18.138	1.00 20.02	F
						85.213	28.548	22.213	1.00 20.47	F
ATOM	5919	C	GIW		6				1.00 18.48	F
ATOM	5920	0	GLN		6	86.243	29.204	22.099		F
ATOM	5921	N	PRO		7	85.229	27.256	22.575	1.00 21.16	
ATOM	5922	CD.	PRO		7	84.071	26.494	23.084	1.00 20.59	F
MOTA	5923	CA	PRO		7	86.471	26.520	22.813	1.00 21.61	F
ATOM	5924	CB	PRO		7	86.037	25.444	23.797	1.00 23.40	F
MOTA	5925	CG	PRO	F	7	84.649	25.123	23.311	1.00 19.67	F
ATOM	5926	C	PRO	F	7	86.996	25.897	21.521	1.00 23.00	F
ATOM	5927	0	PRO	F	7	86.219	25.601	20.610	1.00 23.19	F
MOTA	5928	N	GLU	F	8	88.312	25.714	21.438	1.00 21.78	F
MOTA	5929	CA	GLŪ	F	8	88.904	25.068	20.279	1.00 23.12	f
ATOM	5930	CB	GLU	F	8	90.297	25.632	19.968	1.00 24.50	f
MOTA	5931	CG	GLU	P	8	91.086	24.834	18.915	1.00 26.16	F
ATOM	5932	CD	GLU	F	8	90.360	24.697	17.576	1.00 31.57	F
ATOM	5933		GLU	F	8	89.250	24.114	17.540	1.00 33.65	F
MOTA	5934		GTO		8	90.903	25.171	16.555	1.00 30.66	F
ATOM	5935	C	GTA		8	89.005	23.608	20.680	1.00 22.95	F
MOTA	5936	ō	GTA		8	89.289	23.292	21.833	1.00 23.25	F
		N	LEU		9	88.756	22.712	19.741	1.00 24.74	F
ATOM	5937				9	88.815	21.292	20.047	1.00 27.30	P
MOTA	5938	CA	LEU				20.549	19.272	1.00 25.73	F
MOTA	5939	CB	PEA		9	87.729			1.00 25.73	
ATOM	5940	CG	LEU		9	86.302	21.051	19.494		F
MOTA	5941		LEU		9	85.338	20.235	18.645	1.00 28.18	F
ATOM	5942		LEU		9	85.938	20.943	20.967	1.00 29.61	F
MOTA	5943	C	LEU		9	90.178	20.707	19.712	1.00 28.17	F
ATOM	5944	0	PEA	F	9	90.715	20.940	18.631	1.00 26.94	F
MOTA	5945	N	PRO	F	10	90.765	19.947	20.647	1.00 30.38	F
MOTA	5946	CD	PRO	F	10	90.365	19.707	22.044	1.00 30.47	P
ATOM	5947	CA	PRO	F	10	92.076	19.355	20.370	1.00 34.24	F
ATOM	5948	CB	PRO	F	10	92.556	18.915	21.752	1.00 32.97	F
MOTA	5949	CG	PRO	F	10	91.282	18.561	22.448	1.00 31.98	F
MOTA	5950	С	PRO		10	91.985	18.188	19.393	1.00 35.94	F
ATOM	5951	ō	PRO		10	90.993	17.461	19.376	1.00 38.70	F
ATOM	5952	N	TYR		11	93.016	18.031	18.570	1.00 37.40	F
ATOM	5953	CA	TYR		11	93.075	16.936	17.609	1.00 38.84	P
ATOM	5954	CB	TYR		11	92.126	17.176	16.434	1.00 38.73	F
		CG	TYR		11	92.017	15.969	15.539	1.00 39.56	P
ATOM	5955					91.294	14.848	15.942	1.00 39.88	F
MOTA	5956		TYR		11			15.164	1.00 39.49	F
ATOM	5957		TYR		11	91.254	13.697			P
ATOM	5958				11	92.698	15.913	14.327	1.00 39.73	F
MOTA	5959		TYR		11	92.668	14.765	13.537	1.00 40.44	
MOTA	5960	$\mathbf{cz}$	TYR		11	91,945	13.659	13.964	1.00 40.29	F
MOTA	5961	OH	TYR		11	91.921	12.514	13.200	1.00 40.03	F
MOTA	5962	С	TYR		11	94.498	16.781	17.077	1.00 40.23	F
ATOM	5963	0	TYR		11	95.102	15.708	17.300	1.00 41.88	F
ATOM	5964	OXT	TYR	F	11	94.988	17.742	16.443	1.00 40.58	F
MOTA	5965	0	HOH	H	1	37.560	11.197	17.272	1.00 17.47	H
MOTA	5966	0	HOH	Η	2	81.295	26.543	20.573	1.00 15.95	H
ATOM	5967	0	HOH	H	3	43.884	23.627	16.726	1.00 14.83	H
MOTA	5968	0	HOH	Н	4	89,230	61.015	16.512	1.00 19.10	H
ATOM	5969	0	HOH	H	5	92.090	40.877	18.768	1.00 15.59	H
ATOM	5970	0	HOH		6	57.686	14.054	4.407	1.00 20.02	H
MOTA	5971	0	HOH		7	87.607	31.423	22.217	1.00 11.29	H
ATOM	5972	ō	HOH		В	31.815	41.479	5.673	1.00 23.91	н
ATOM	5973	ŏ	нон		9	46.112	3.594	18.714	1.00 20.15	H
ATOM	5974	ő	HOH		10	86.724	67.786	15.551	1.00 22.39	. н
		Ö	HOH		11	42.599	14.833	17.213	1.00 16.12	н
MOTA	5975					93.679	37.081	11.737	1.00 15.03	H
MOTA	5976	0	HOH		12		0.581	25.262	1.00 13.69	н
MOTA	5977	0	HOH		13	50.288				н
MOTA	5978	0	HOH		14	96.256	37.853	25.291	1.00 12.90	
MOTA	5979	0	HOH		15	90.711	30.936	37.307	1.00 31.88	H
ATOM	5980	0	HOH		16	80.045	39.846	25.144	1.00 33.11	H
MOTA	5981	0	HOH		17	80.708	45.662	11.514	1.00 41.56	H
MOTA	5982	0	HOH		18	42.215	0.119	11.193	1.00 15.83	H
ATOM	5983	0	HOH		19	95.828	50.485	5.930	1.00 27.67	H
MOTA	5984	0	HOE		20	48.809	37.278	14.928	1.00 36.10	H
ATOM	5985	0	HOH	H	21	47.553	-0.403	11.823	1.00 14.62	H
ATOM	5986	0	HOH	н	22	94.554	76.132	19.122	1.00 83.80	H
MOTA	5987	0	HOH	н	23	83.295	48.460	17.328	1.00 17.64	H
ATOM	5988	0	HOH		24	88.976	42.102	7.818	1.00 26.11	H
MOTA	5989	0	HOH		25	99.041	56.322	24.823	1.00 24.86	H
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ATOM	5990	0	нон н	26	47.640	0.006	20.312	1.00 18.95	H
ATOM	5991	0	нон н	27	46.987	29.359	11.916	1.00 21.84	H
MOTA	5992	ō	нон н	28	88.283	37.229	11.279	1.00 21.34	н
							36.424		
MOTA	5993	0	нон н	29	49.878	-9.043		1.00 32.47	H
MOTA	5994	0	нон н	30	82.777	39.366	24.935	1.00 24.79	.H
MOTA	5995	0	нон н	31	72.919	25.704	15.123	1.00 18.09	H
MOTA	5996	0	нон н	32	86.830	25.153	13.558	1.00 24.14	H
ATOM	5997	o	нон н	33	43.152	5.651	13.774	1.00 19.96	H
						27.732	5.367	1.00 34.73	H
ATOM	5998	0	нон н	34	100.654				
MOTA	5999	0	нон н	35	48.550	32.122	26.894	1.00 20.17	H
ATOM	6000	0	нон н	36	78.728	36.578	6.822	1.00 32.92	H
ATOM	6001	0	нон н	37	89.361	11.980	24.953	1.00 51.75	H
MOTA	6002	ō	нон н	38	90.411	24.657	31.926	1.00 28.29	H
							8.462	1.00 22.43	н
ATOM	6003	0	нон н	39	80.690	24.233			
MOTA	6004	0	нон н	40	83.769	65.973	-5.489	1.00 21.06	H
MOTA	6005	0	нон н	41	87.710	34.692	7.008	1.00 22.47	Н
ATOM	6006	0	HOH H	42	38.997	4.521	15.299	1.00 25.36	H
MOTA	6007	0	нон н	43	94.223	46.644	24.674	1.00 32.67	H
MOTA	6008	ō	нон н	44	35.150	15.757	26.294	1.00 29.03	н
ATOM	6009	0	нон н	45	85.059	24.652	18.280	1.00 25.63	H
MOTA	6010	0	нон н	46	67.739	6.320	18.991	1.00 43.67	H
MOTA	6011	0	нон н	47	92.376	63.977	12.866	1.00 32.46	H
MOTA	6012	0	HOH H	48	91.526	49.479	22.504	1.00 29.70	H
ATOM	6013	Ō	нон н	49	56.333	-2.088	24.733	1.00 28.53	H
			нон н		100.482	53.937	3.942	1.00 52.26	н
MOTA	6014	0		50					
MOTA	6015	0	нон н	51	48.244	18.753	22.918	1.00 44.88	H
ATOM	6016	0	HOH H	52	32.577	-0.558	6.769	1.00 33.70	H
ATOM	6017	0	HOH H	53	47.162	26.527	12.972	1.00 29.72	H
ATOM	6018	0	нон н	54	98.621	66.834	5.100	1.00 52.20	H
ATOM	6019	ō	нон н	55	88.106	52.134	17.293	1.00 21.13	H
								1.00 25.89	H
ATOM	6020	0	нон н	56	59.655	31.307	17.069		
MOTA	6021	0	HOH H	57	73.562	24.323	12.997	1.00 23.51	H
MOTA	6022	0	нон н	58	43.748	32.725	20.165	1.00 52.72	H
ATOM	6023	0	нон н	59	26.392	-7.072	11.400	1.00 26.20	H
ATOM	6024	ō	нон н	60	83.955	73.751	16.805	1.00 18.19	H
		ŏ	нон н	61		-19.766	10.675	1.00 28.79	H
ATOM	6025								
MOTA	6026	0	нон н	62	52.436	38.720	16.630	1.00 28.35	H
MOTA	6027	0	нон н	63	60.555	9.392	19.914	1.00 28.43	н
ATOM	6028	0	нон н	64	62.105	2.197	11.948	1.00 33.33	H
MOTA	6029	0	нон н	65	40.514	-12.059	13.631	1.00 21.32	H
MOTA	6030	ō	нон н	66	65.876	23.972	14.155	1,00 21.11	н
		ō	нон н	67	84.702	18.013	5.666	1.00 19.12	н
ATOM	6031								н
ATOM	6032	0	нон н	68	64.715	11.655	15.936	1.00 28.72	
MOTA	6033	0	нон н	69	85.418	74.949	14.820	1.00 27.90	H
MOTA	6034	0	нон н	70	77.974	25.419	23.038	1.00 42.15	H
MOTA	6035	0	нон н	71	65.805	8.484	20.741	1.00 44.01	H
MOTA	6036	0	нон н	72	51.276	26.045	10.800	1.00 28.36	H
		ŏ	нон н	73	65.226	22.195	25.831	1.00 36.11	н
MOTA	6037							1.00 53.81	н
ATOM	6038	0	нон н	74	101.567	46.068	1.107		
MOTA	6039	0	нон н	75	32.615	31.234	1.517	1.00 21.03	H
MOTA	6040	0	нон н	76	42.100	-0.001	13.802	1.00 23.44	H
ATOM	6041	0	нон н	77	35.124	40.614	14.668	1.00 27.61	H
ATOM	6042	0	нон н	78	92.548	46.813	7.595	1.00 31.64	H
MOTA	6043	ŏ	нон н	79	34.670	13.941	14.778	1.00 22.87	н
						27.671	28.270	1.00 42.07	н
ATOM	6044	0	нон н	80	98.527				
MOTA	6045	0	нон н	81	30.588	36.032	16.540	1.00 37.52	H
ATOM	6046	0	нон н	82	89.345	42.957	13.940	1.00 22.73	H
ATOM	6047	0	нон н	83	92.891	18.085	10.698	1.00 32.35	H
ATOM	6048	0	нон н	84	90.050	48.556	16.519	1.00 27.30	H
MOTA	6049	o	нон н	85	110.812	49.549	15.813	1.00 27.68	H
						21.668	2.499	1.00 39.37	н
ATOM	6050	0	нон н	86	75.872				
MOTA	6051	0	нон н	87	52.567	14.010	7.270	1.00 34.20	H
MOTA	6052	0	нон н	88	69.016	32.569	12.651	1.00 36.96	H
MOTA	6053	0	нон н	89	96.637	25.945	31.742	1.00 37.26	H
ATOM	6054	o	нон н	90		-12.998	8.560	1.00 22.82	н
	6055	ŏ	нон н	91	113.021	48.469	17.945	1.00 47.59	н
MOTA							23.930	1.00 31.02	H
MOTA	6056	0	нон н	92	34.266	25.052			
MOTA	6057	0	нон н	93	51.464	31.946	19.300	1.00 15.75	H
MOTA	6058	0	нон н	94	80.054	50.912	15.041	1.00 25.94	H
ATOM	6059	0	нон н	95	40.413	-13.432	16.393	1.00 39.73	H
ATOM	6060	0	нон н	96	57.701		7.708	1.00 25.27	H
MOTA	6061	ō	нон н	97	80,838		26.436	1.00 27.67	H
					58.205	13.023	20.294	1.00 27.57	н
MOTA	6062	0	нон н	98					
ATOM	6063	0	нон н	99	41.832	30.497	15.601	1.00 27.32	H

ATOM	6064	0	HOH H 100	72.807	29.880	11.618	1.00 28.05	H
ATOM	6065	o	HOH H 101	48.499	5.079	4.053	1.00 38.72	H
MOTA	6066	0	нон н 102	100.679	66.408	9.019	1.00 36.21	H
ATOM	6067	0	HOH H 103	45.023	41.442	11.747	1.00 42.72	H
MOTA	6068	0	HOH H 104	83.296	63.483	-2.738	1.00 27.46	H
MOTA	6069	ō	HOH H 105	85.067	29.522	34.732	1.00 35.62	H
MOTA	6070	0	HOH H 106	72.272	53.390	15.314	1.00 38.75	H
MOTA	6071	0	HOH H 107	80,600	27.688	5.225	1.00 26.04	H
ATOM	6072	o	HOH H 108	71.251	18.567	16.503	1.00 29.08	Н
MOTA	6073	0	HOH H 109	88.274	65.356	19.510	1.00 26.70	H
MOTA	6074	0	HOH H 110	43.031	4.836	7.813	1.00 38.59	H
ATOM	6075	0	HOH H 111	101.304	35.384	4.755	1.00 43.53	H
ATOM	6076		HOH H 112	44.554	10.725	19.619	1.00 21.38	н
		0						
MOTA	6077	0	HOH H 113	115.506	34.478	5.615	1.00 46.62	H
MOTA	6078	0	HOH H 114	36.124	-25.634	9.802	1.00 42.69	H
MOTA	6079	0	нон н 115	34.494	-33.304	20.170	1.00 61.12	H
MOTA	6080	0	HOH H 116	38.663	26.161	-2.715	1.00 31.39	H
ATOM	6081	0	HOH H 117	105.197	41.384	18.739	1.00 38.53	H
MOTA	6082	0	HOH H 118	38.437	-12.372	18.422	1.00 32.47	H
MOTA	6083	ō	HOH H 119	45.430	15.732	9.556	1.00 32.39	н
MOTA	6084	0	HOH H 120	70.475	9.817	-1.029	1.00 53.38	H
MOTA	6085	0	HOH H 121	87.895	64.540	22.445	1.00 47.01	H
MOTA	6086	0	HOH H 122	39.337	36.650	16.644	1.00 25.21	H
MOTA	6087	ō	HOH H 123	104.091	50.783	20.204	1.00 31.31	н
MOTA	6088	0	HOH H 124	72.528	13.825	20.909	1.00 62.81	H
ATOM	6089	0	HOH H 125	55.353	-5.411	5.747	1.00 25.46	H
MOTA	6090	0	HOH H 126	97.848	63.704	25.177	1.00 27.84	H
			HOH H 127					
MOTA	6091	0		89.799	75.117	14.074	1.00 49.56	H
MOTA	6092	0	HOH H 128	96.226	35.565	0.211	1.00 40.25	H
MOTA	6093	0	HOH H 129	25.125	-15.445	19.161	1.00 37.04	H
ATOM	6094	o	HOH H 130	90.627	52.974	9.649	1.00 22.70	H
ATOM	6095	0	HOH H 131	114.398	29.773	11.425	1.00 42.36	H
MOTA	6096	0	HOH H 132	69.810	89.608	-0.164	1.00 53.48	H
MOTA	6097	0	HOH H 133	99.069	30.421	4.728	1.00 31.21	H
MOTA	6098	0	HOH H 134	37,335	49.129	5.746	1.00 43.90	H
MOTA	6099	0	HOH H 135	77.753	73.821	17.600	1.00 50.43	H
MOTA	6100	0	HOH H 136	44.853	33.208	11.090	1.00 21.26	н
MOTA	6101	0	HOH H 137	88.697	80.608	-4.574	1.00 49.42	H
ATOM	6102	0	HOH H 138	62.018	-6.136	9.010	1.00 30.19	H
MOTA	6103	0	нон н 139	35.964	-5.810	5.494	1.00 45.47	H
MOTA	6104	0	HOH H 140	73.968	65.480	8.013	1.00 43.93	Н
MOTA	6105	0	HOH H 141	78.361	66.868	24.455	1.00 57.76	H
ATOM	6106	0	HOH H 142	53.527	3.199	22.332	1.00 32.95	H
MOTA	6107	0	нон н 143	56.018	-6.530	25.205	1.00 42.75	H
ATOM	6108	0	HOH H 144	82.930	52.617	28.345	1.00 32.35	H
MOTA	6109	0	HOH H 145	28.607	-21.313	24.210	1.00 48.87	H
MOTA	6110	0	HOH H 146	86.079	41.197	35.698	1.00 36.97	H
			HOH H 147		8.399		1.00 32.21	H
ATOM	6111	0		35.017		11.516		
ATOM	6112	0	HOH H 148	25.864	-19.905	17.166	1.00 41.53	H
MOTA	6113	0	HOH H 149	55.504	20.659	6.959	1.00 36.63	H
MOTA	6114	0	HOH H 150	106.046	47.260	19.571	1.00 30.60	H
ATOM	6115	ō		108.769	26.147	5.447	1.00 48.82	H
		_	HOH H 151					
MOTA	6116	0	нон н 152	38.689	17.576	4.331	1.00 39.07	H
MOTA	6117	0	HOH H 153	97.787	62.580	8.740	1.00 29.61	H
MOTA	6118	0	HOH H 154	59.501	-12.817	20.769	1.00 50.36	H
MOTA	6119	0	нон н 155	47.887	40.072	-4.641	1.00 51.05	H
MOTA	6120	0	HOH H 156	60.057	16.564	27.477	1.00 40.66	H
MOTA	6121	0	HOH H 157	67.048	27.841	20.873	1.00 39.66	H
ATOM	6122	0	нон н 158	37.028	32.932	18.669	1.00 37.23	H
							1.00 46.64	
MOTA	6123	0	нон н 159	121.780		-3.076		Н
MOTA	6124	0	HOH H 160	39.196		27.271	1.00 29.99	H
MOTA	6125	0	HOH H 161	113.285	44.237	19.561	1.00 39.04	H
MOTA	6126	0	нон н 162	43.379		19.370	1.00 27.58	H
			нон и 163	91.636		11.885	1.00 54.73	H
MOTA	6127	0						
MOTA	6128	0	HOH H 164	113.381		20.020	1.00 54.22	Н
ATOM	6129	0	HOH H 165	79.238	62.082	24.112	1.00 36.07	H
ATOM	6130	0	нон н 166	27.985		18.424	1.00 36.25	н
ATOM	6131	ō	HOH H 167		-10.661	20.615	1.00 9.89	н
MOTA	6132	0	HOH H 168	93.577		20.182	1.00 14.03	H
MOTA	6133	0	нон н 169	97.912	51.662	7.309	1.00 24.22	H
ATOM	6134	0	нон н 170	69.616	4.375	18.521	1.00 38.01	H
MOTA	6135	ō	нон н 171	80.870		6.002	1.00 21.84	н
								н
MOTA	6136 6137	0	нон н 172	50.564		5.906	1.00 32.25	
MOTA			HOH H 173	88.207	37.288	13.919	1.00 19.68	H

ATOM	6138	0	HOH H 174	93.800	47.651	27.174	1.00 41.65	H
MOTA	6139	0	HOH H 175	52.842	0.304	25.210	1.00 28.07	H
MOTA	6140	0	HOH H 176	66.457	4.742	14.051	1.00 28.64	H
MOTA	6141	0	HOH H 177	36.948	12.416	15.109	1.00 28.66	H
MOTA	6142	0	HOH H 178	103.292	41.793	7.607	1.00 28.51	н
ATOM	6143	0	HOH H 179	86.476	36.035	9.339	1.00 27.43	H
ATOM	6144	ō	HOH H 180	82.262	41.159	26.845	1.00 24.13	н
ATOM	6145	ō	HOH H 181	32.348	15.030	26.400	1.00 30.06	H
ATOM	6146	ŏ	HOH H 182	69.916	30.709	14.482	1.00 42.81	н
MOTA	6147	o	HOH H 183	48.060	10.142	26.751	1.00 49.12	H
ATOM		o	HOH H 184	45.863	-9.131	37.252	1.00 43.70	н
	6148		HOH H 185	32.095	-3.806	34.251	1.00 41.46	Н
ATOM	6149	0	HOH H 186			8.914	1.00 33.62	н
MOTA	6150	0		108.258	31.975 64.293	8.210		
ATOM	6151	0	HOH H 187	99.465			1.00 54.43	H
ATOM	6152	0	HOH H 188	74.677	30.785	27.841	1.00 28.20	H
MOTA	6153	0	HOH H 189	44.953	0.968	35.892	1.00 32.25	H
ATOM	6154	0	HOH H 190	88.523	27.792	36.268	1.00 30.83	H
MOTA	6155	0	нон н 191	37.736	8.611	11.729	1.00 38.92	H
MOTA	6156	0	нон н 192	35.988	45.178	12.964	1.00 33.85	H
ATOM	6157	0	HOH H 193	77.222	68.027	1.401	1.00 27.02	H
ATOM	6158	0	HOH H 194	63.326	-8.764	15.926	1.00 38.46	H
ATOM	6159	0	нон н 195	109.635	61.489	27.644	1.00 52.79	H
ATOM	6160	0	HOH H 196	101,299	67.528	11.319	1.00 38.92	H
ATOM	6161	0	нон н 197	77.295	56.116	25.768	1.00 36.83	H
ATOM	6162	0	нон н 198	81.538	22.288	0.320	1.00 47.08	Н
ATOM	6163	0	HOH H 199	55.989	3.900	0.756	1.00 46.35	H
MOTA	6164	0	HOH H 200	66.200	40.514	17.513	1.00 43.54	H
ATOM	6165	0	HOH H 201	40.497	-1.046	9.238	1.00 27.84	H
ATOM	6166	0	HOH H 202	57.171	27.504	8.258	1.00 52.74	H
ATOM	6167	0	HOH H 203	44.592	-6.430	37.531	1.00 37.55	H
ATOM	6168	0	HOH H 204	26.892	-1.642	9.494	1.00 55.58	H
ATOM	6169	0	HOH H 205	83.350	58.389	2.759	1.00 46.24	H
ATOM	6170	0	нон н 206	112.353	45.284	9.770	1.00 30.99	H
MOTA	6171	0	HOH H 207	86.315	23.927	16.100	1.00 41.36	H
MOTA	6172	0	HOH H 208	67.053	45.396	12.396	1.00 31.02	н
ATOM	6173	0	нон н 209	111.609	60.418	8.362	1.00 52.01	H
ATOM	6174	0	HOH H 210	91.254	47.553	32.752	1.00 41.71	H
MOTA	6175	0	HOH H 211	88.489	39.944	11.117	1.00 34.00	н
ATOM	6176	0	HOH H 212	104.972	69.233	16.415	1.00 37.26	H
ATOM	6177	o	HOH H 213	23.462	39.893	6.692	1.00 56.45	H
MOTA	6178	ō	HOH H 214	84.114	54.447	-1.718	1.00 42.58	H
ATOM	6179	ō	HOH H 215	105.045	66.068	22.775	1.00 24.48	н
ATOM	6180	ō	нон н 216	85.378	52.388	17.025	1.00 37.91	H
MOTA	6181	ō	HOH H 217	91.411	30.837	4.259	1.00 23.59	H
ATOM	6182	ŏ	HOH H 218	99.019	37.803	25.178	1.00 37.20	H
ATOM	6183	ō	HOH H 219	88.866	41.183	35.781	1.00 42.88	H
MOTA	6184	ŏ	HOH H 220	66.946	25.931	12.530	1.00 45.53	H
ATOM	6185	ō	HOH H 221	83.809	61.544	-0.645	1.00 32.51	н
ATOM	6186	ŏ	HOH H 222	91.766	28.386	3.286	1.00 29.97	н
ATOM	6187	ō	нон н 223	83.302	45.674	11.423	1.00 40.65	н
ATOM	6188	o	HOH H 224	59.198	3.628	18.904	1.00 22.61	н
ATOM	6189	o	HOH H 225		-11.852	5.930	1.00 29.77	н
ATOM	6190	o	HOH H 226	88.953	22.712	24.560	1.00 23.54	н
MOTA	6191	ŏ	HOH H 227	108.379	54.102	21.160	1.00 30.79	н
ATOM		0	HOH H 228	44.957	16.820	6.827	1.00 37.14	н
MOTA	6192			105.872	50.217	22.393	1.00 37.11	н
	6193	0	нон н 229	40.390	52.287	-1.729	1.00 62.00	н
ATOM	6194	0	нон н 230	103.837	27.586		1.00 50.76	H
ATOM	6195	0	HOH H 231			24.806	1.00 40.65	н
ATOM	6196	0	нон н 232	50.931	9.397 2.382	25.207	1.00 46.98	. н
ATOM	6197	0	нон н 233	64.739		27.973		н
ATOM	6198	0	нон н 234	38.363	0.460	8.402	1.00 28.58	н
MOTA	6199	0	HOH H 235	73.577	50.129	18.561	1.00 36.68	H
ATOM	6200	0	нон н 236	100.912	58.519	6.876	1.00 36.99	H
ATOM	6201	0	нон н 237	100.664	26.841	26.380	1.00 36.27	
MOTA	6202	0	нон н 238	82.528	48.080	12.484	1.00 44.97	H
ATOM	6203	0	нон н 239	70.870	44.782	13.746	1.00 26.53	H
ATOM	6204	0	HOH H 240	71.914	-9.049	17.302	1.00 59.29	H
ATOM	6205	0	HOH H 241	28.024	9.146	32.377	1.00 43.91	H
MOTA	6206	0	HOH H 242	55.531	-2.470	4.880	1.00 50.20	H
MOTA	6207	0	HOH H 243	63.362	16.623	21.334	1.00 30.95	H
ATOM	6208	0	HOH H 244	71.813	27.548	12.914	1.00 54.77	H
MOTA	6209	0	HOH H 245	22.793	-3.930	12.731	1.00 39.10	H
ATOM	6210	0	нон н 246	73.087	44.091	34.124	1.00 47.86	H
MOTA	6211	0	HOH H 247	48.717	31.774	19.850	1.00 33.46	н

3 most	C010	^	11011 II 240	100 051	61 210	7 741	1.00 35.49	н
MOTA	6212	0	HOH H 248	100.851	61.218	7.741		
MOTA	6213	0	HOH H 249	116.291	47.311	12.227	1.00 49.67	H
MOTA	6214	0	HOH H 250	99.469	40.748	22.418	1.00 25.82	H
MOTA	6215	0	HOH H 251	52,271	4.031	24.614	1.00 44.68	н
MOTA	6216	ō	HOH H 252	106.629	40.298	32.271	1.00 59.44	H
					-9.303	3.049	1.00 26.81	H
MOTA	6217	0	нон н 253	45.587				
MOTA	6218	0	HOH H 254	52.547	-9.432	27.670	1.00 45.08	H
MOTA	6219	0	HOH H 255	75.854	21.157	27.640	1.00 42.33	H
ATOM	6220	0	нон н 256	82.119	63.444	23.430	1.00 37.84	H
			нон н 257	104.091	38.660	18.936	1.00 30.29	н
MOTA	6221	0						
MOTA	6222	0	нон н 258	79.477	56.121	8.190	1.00 39.16	H
ATOM	6223	0	HOH H 259	101.351	32.257	5.631	1.00 29.94	H
MOTA	6224	0	HOH H 260	93.989	23.313	31.488	1.00 35.30	н
ATOM	6225	0	HOH H 261	28.754	-1.723	6.977	1.00 36.90	H
			HOH H 262	93.007	48.370	9.901	1.00 49.06	H
ATOM	6226	0						
MOTA	6227	0	нон н 263	82.990	88.137	9.529	1.00 39.70	H
MOTA	6228	0	HOH H 264	118.031	51.582	0.542	1.00 36.21	H
ATOM	6229	0	HOH H 265	21.682	15.046	11.602	1.00 62.29	H
MOTA	6230	0	нон н 266	34.210	24.576	5.314	1.00 18.89	н
				85.829		14.911	1.00 25.26	н
MOTA	6231	0	нон н 267		40.095			
ATOM	6232	0	нон н 268	102.070	38.308	21.059	1.00 41.79	H
MOTA	6233	0	HOH H 269	41.071	-2.346	7.039	1.00 38.87	H
ATOM	6234	0	HOH H 270	68.717	3.686	16.083	1.00 37.79	н
ATOM	6235	ō	HOH H 271		-12.649	12.753	1.00 29.26	н
						4.145		H
MOTA	6236	0	нон н 272	36.426	24.744		1.00 45.88	
ATOM	6237	0	HOH H 273	88.670	31.858	5.525	1.00 39.43	H
ATOM	6238	0	HOH H 274	90.819	38.524	36.028	1.00 30.15	H
ATOM	6239	0	нон н 275	90.790	49.861	10.317	1.00 39.97	н
	6240	ō	HOH H 276	77.026	11.969	13.970	1.00 44.87	H
ATOM							1,00 40.47	H
ATOM	6241	0	HOH H 277	36.555	12.078	12.344		
ATOM	6242	0	HOH H 278	52.331	7.302	24.972	1.00 49.30	H
MOTA	6243	0	HOH H 279	92.612	33.229	3.564	1.00 40.55	H
ATOM	6244	0	HOH H 280	83.546	64.142	25.612	1.00 50.28	H
ATOM	6245	ō	HOH H 281	28.206	-1.891	36.868	1.00 44.06	H
								н
MOTA	6246	0	нон н 282	93.185	20.914	30.917	1.00 44.51	
ATOM	6247	0	HOH H 283	98.176	41.763	24.500	1.00 44.20	H
MOTA	6248	0	HOH H 284	29.174	-0.123	4.304	1.00 46.75	H
MOTA	6249	0	HOH H 285	79,206	77.643	14.919	1.00 30.21	Н
ATOM	6250	ō	нон н 286	90.531	26.085	37.436	1.00 36.96	н
						21.054	1.00 49.55	н
ATOM	6251	0	нон н 287	55.726	0.396			
MOTA	6252	0	HOH H 288	111.246	30.915	19.699	1.00 42.91	H
ATOM	6253	0	HOH H 289	77.000	58.921	5.300	1.00 47.04	, Н
ATOM	6254	Ο,	HOH H 290	34.339	-9.458	5.288	1.00 25.50	H
MOTA	6255	o	нон н 291	109.784	29.168	15.534	1.00 45.96	н
				93.674	48.853	29.650	1.00 48.76	н
ATOM	6256	0	нон н 292					
MOTA	6257	0	нон н 293	92.299	47.066	3.801	1.00 37.41	H
MOTA	6258	0	HOH H 294	110.965	23.141	11.799	1.00 42.97	H
ATOM	6259	0	HOH H 295	90.562	45.235	33.919	1.00 33.83	н
ATOM	6260	ō	нон н 296		-10.500	25.018	1.00 49.78	н
						11.362	1.00 54.22	H
MOTA	6261	0	нон н 297	54.676	36.195			
ATOM	6262	0	нон н 298	107.263	59.234	5.282	1.00 56.05	H
ATOM	6263	0	нон н 299	70.560	48.918	1.476	1.00 49.72	H
ATOM	6264	0	нон н 300	84.037	38.916	5.971	1.00 39.33	H
MOTA	6265	ō	нон н 301	86.468	41.381	11.971	1.00 45.69	H
				24.400	11.569	23.610	1.00 36.73	H
ATOM	6266	0	нон н 302					
ATOM	6267	0	HOH H 303	73.087	79.808	7.028	1.00 46.20	H
MOTA	6268	0	HOH H 304	72.681	43.116	14.941	1.00 51.84	H
MOTA	6269	0	нон н 305	84.844	42.198	15.611	1.00 26.23	н
ATOM	6270	0	нон н 306	54.135	19.007	24.978	1.00 27.41	H
			нон н 307	67.044	10.459	18.465	1.00 44.92	H
ATOM	6271	0						
MOTA	6272	0	нон н 308	82.262	49.436	14.864	1.00 39.04	. н
ATOM	6273	0	нон н 309	114.093	50.994	16.895	1.00 43.32	H
MOTA	6274	0	нон н 310	64.428	3.092	30.590	1.00 43.29	H
ATOM	6275	o	HOH H 311	81.152	70.187	18.656	1.00 34.21	H
ATOM	6276	Ö	нон н 312	74.596	81.584	-2.515	1.00 55.00	H
						22.464	1.00 32.98	H
MOTA	6277	0	нон н 313	61.161	25.774			
MOTA	6278	0	HOH H 314	53.149	-7.019	4.754	1.00 26.01	H
ATOM	6279	0	HOH H 315	44.571	8.317	33.567	1.00 40.32	H
ATOM	6280	0	нон н 316	82.293	49.769	10.587	1.00 35.22	H
ATOM	6281	ō	нон н 317	48.467	8.859	24.614	1.00 42.38	H
				56.588	-8.027	4.728	1.00 44.65	н
MOTA	6282	0	HOH H 318				1.00 42.45	
MOTA	6283	0	нон н 319		-23.239	26.551		H
MOTA	6284	0	нон н 320	82.483		7.719	1.00 39.22	H
ATOM	6285	0	HOH H 321	82.063	19.937	23.440	1.00 35.69	H

106.025 63.366 22.616 1.00 31.93 ATOM 6286 HOH H 322 H 9.890 8.669 1.00 38.11 ATOM 6287 0 HOH H 323 46,181 H 75.56B 6.998 1.00 41.82 ATOM 6288 0 HOH H 324 71.708 H 6289 HOH H 325 108.280 34.405 3.851 1.00 30.72 н ATOM ٥ 1.00 40.72 MOTA 6290 0 HOH H 326 32.275 40.921 14.635 H 15.785 5.690 1.00 42.29 Н 0 37.556 ATOM 6291 HOH H 327 37.182 1.00 31.78 MOTA 6292 0 HOH H 328 85.569 33.598 н 0 HOH H 329 33.070 -11.287 23.137 1.00 48.90 H ATOM 6293 нон н 330 87.593 16.513 19.683 1.00 45.53 ATOM 6294 0 H HOH H 331 53.631 17.853 1.00 39.81 MOTA 6295 0 116.176 ATOM 6296 0 HOH H 332 26.940 -11.377 14.930 1.00 39.40 H 60.033 22.456 1.00 32.84 ATOM 6297 0 нон н 333 28.679 H 52.472 15.182 2.562 1.00 48.72 н MOTA 6298 0 HOH H 334 H 84.377 54.588 4.646 1.00 40.99 ATOM 6299 0 HOH H 335 115.759 67.454 19.970 1.00 46.15 H ATOM 6300 HOH H 336 H MOTA 6301 0 HOH H 337 88.969 52.684 25.112 1.00 42.31 36.351 12.852 9.875 1.00 37.11 н 0 HOH H 338 ATOM 6302 1.00 49.82 н MOTA 6303 ٥ HOH H 339 97.702 31.578 2.653 HOH H 340 53.964 -6.543 26.981 1.00 35.52 H MOTA 6304 0 24.475 -17.438 ATOM 6305 0 HOH H 341 17.094 1.00 38.04 н 58.530 0.915 19.036 1.00 43.08 H HOH H 342 6306 0 ATOM 39.025 н 77.156 37.203 1.00 48.54 ATOM 6307 0 HOH H 343 H ATOM 6308 HOH H 344 49.978 -1.361 0.435 1.00 39.48 6309 0 HOH H 345 53.900 37.104 13.703 1.00 47.74 н ATOM 13.575 1.00 57.13 H HOH H 346 77.886 49.625 ATOM 6310 0 Н 0.570 1.00 50.38 MOTA 6311 0 **HOH H 347** 57.053 8.721 ATOM 6312 0 HOH H 348 96.803 63.745 10.854 1.00 41.14 H 89.009 70.808 11.906 1.00 45.67 Н 0 HOH H 349 ATOM 6313 1.00 42.47 н 22.353 8.221 66.363 MOTA 6314 ٥ HOH H 350 6315 0 HOH H 351 52.578 25.044 8.541 1.00 41.16 H ATOM 81.789 73.640 -3.536 1.00 50.48 н MOTA 6316 HOH H 352 Н 67.632 -11.181 13.891 1.00 48.24 MOTA 6317 0 HOH H 353 22.367 1.00 14.47 41.357 -5.652 ATOM 6318 0 HOH H 354 G 6319 C1 EDO G 501 37.685 -5.096 30.876 1.00 23.96 MOTA 38.224 -4.213 31.883 1.00 23.38 G MOTA 6320 01 EDO G 501 EDO G 501 38.742 -6.046 30.406 1.00 25.29 G 6321 C2 ATOM G 39.062 -6.931 31.464 1.00 26.30 EDO G 501 ATOM 6322 02 89.146 26.377 27.000 1.00 41.69 MOTA 6323 C1 EDO G 502 G 88.631 26.508 28.343 1.00 51.10 ATOM 6324 01 EDO G 502 1.00 43.14 G EDO G 502 88.436 25.261 26.303 ATOM 6325 C2 88.726 24.052 26.967 1.00 41.73 MOTA 6326 02 EDO G 502 G 30.633 1.00 21.00 6327 C1 **EDO G 503** 85.093 31.920 ATOM G MOTA 6328 01 **EDO G 503** 85.283 30.597 31,203 1.00 18.65 31.186 1.00 19.69 G C2 EDO G 503 83.846 32.561 6329 MOTA 84.148 33.101 32.454 1.00 20.94 G EDO G 503 MOTA 6330 02 1.00 38.01 25.885 34.956 3.907 MOTA 6331 C1 **EDO G 504** G 1.00 36.69 EDO . G 504 33.976 2.838 25.869 ATOM 6332 01 EDO G 504 36.360 3.344 25.982 1.00 39.84 G MOTA 6333 C2 36.573 2.396 24.935 1.00 33.51 **KDO G 504** ATOM 6334 02 END

## Example 4

Binding of altered gluten peptides (peptide analogs) to MHC molecules is assayedwith purified HLA molecules. Binding of labeled peptide to purified HLA DQ2 molecules can be measured as described by Johansen et al. (1996) Int Immmunol (8), 177-82. Briefly, purified DQ2 molecules (50 - 1000 nM) are incubated with the 125-I radiolabeled indicator peptide (MB 65kDa 243-255Y, sequence KPLLIIAEDVEGEY; 20 000 cpm, 1-5 nM) at pH 4.9. After incubation for 24 hours, the peptide bound to DQ2 and the non-bound peptide are separated on Sephadex G25 superfine spun columns. The radioactivity in the bound and non-bound fractions was counted in a gamma-counter, and the fraction of peptide bound to DQ2 (cpm in the bound fraction/total cpm recovered) is calculated. The binding capacities of the peptide binding inhibitors are assayed by testing their ability to inhibit the binding of the labeled indicator peptide. The concentration required to give 50%

inhibition (IC $_{50}$ ) is calculated. Since the level of IC $_{50}$  may vary between separate titration experiments, the IC $_{50}$  values are compared to the IC $_{50}$  of a reference peptide by determining the relative binding capacity (RBC), which is the ratio: IC $_{50}$  of reference peptide / IC $_{50}$  of test compound. HLA-DQ2 molecules can be isolated by antibody affinity chromatography from lysates of HLA-DQ2 homozygous Epstein Barr virus transformed B-lymphoblastoid cell lines (detergent solubilized) or from water soluble, recombinant molecules produced similarly as described in Example 3 above. The recombinant molecules can be made with or without covalently linked peptide and with a biotin recognition sequence at the C-terminal end of the  $\beta$ -subunit that facilitates adsorption of HLA-DQ2 to several streptavidin coated supports, thereby enabling alternative ways for measurement of IC $_{50}$ . A peptide analog with an IC $_{50}$  value of less than 100  $\mu$ M is suitable for further screenings.

[92] Alternatively, binding of altered gluten peptides to HLA-DQ2 can also be assayed using the soluble DQ2 heterodimer produced as described in Example 3 above. The presence of the biotin recognition sequence at the C-terminal end of the β-subunit facilitates adsorption of HLA-DQ2 to several streptavidin coated supports, thereby enabling measurement of IC<sub>50</sub> or K<sub>i</sub>.

Candidate peptide analogs are further tested for their ability to inhibit proliferation of [93] T cells specific for gluten peptides. This is done by using HLA-DQ2 restricted T cell clones (TCC) and glutaraldehyde fixed antigen presenting cells (e.g. Epstein Barr virus transformed B-lymphoid transformed cells) expressing HLA-DQ2. The antigen presenting cells are pelleted and resuspended in RPMI containing 0.05% glutaraldehyde for 90 sec, whereafter glycin to a final concentration of 0.2 M is added for 60 sec. The cells are then washed, counted, and resuspended in PBS or PBS buffered with citrate phosphate to a final pH of 4.9. The fixed APC are incubated overnight with various concentrations of peptides. The inhibitory peptides are usually added 30 min prior to the stimulatory peptide. The antigen presenting cells are then washed twice and resuspended in culture medium of RPMI-1640 supplemented with 15% v/v heat inactivated pooled human serum and the T cells are added. The experiments are performed in triplicates of 3-5 X 10<sup>4</sup> TCC with 5 X 10<sup>4</sup> fixed APC and various titrations of inhibitory and stimulatory peptides. Following an incubation period of 48 hours, each culture is pulsed with [3H]-thymidine for an additional 12-18 hours. Cultures are then harvested on fiberglass filters and counted as above. Mean CPM and standard error of the mean are calculated from data determined in triplicate cultures. Peptide analogs that inhibit proliferation to approximately 25% at a concentration of 50 µM or greater are suitable for further screening.

[94] All publications and patent applications cited in this specification are herein incorporated by reference as if each individual publication or patent application were specifically and individually indicated to be incorporated by reference.

[95] Although the foregoing invention has been described in some detail by way of illustration and example for purposes of clarity of understanding, it will be readily apparent to those of ordinary skill in the art in light of the teachings of this invention that certain changes and modifications may be made thereto without departing from the spirit or scope of the appended claims.

## WHAT IS CLAIMED IS:

1. An HLA-binding peptide inhibitor; wherein said inhibitor is an analog of an immunogenic gluten oligopeptide of at least about 8 residues in length, wherein the immunogenic gluten oligopeptide is altered by the replacement of one or more amino acids; and wherein said analog binds tightly to HLA molecules; is proteolytically stable; and does not activate disease-specific T cells.

- The HLA-binding peptide inhibitor of Claim 1, wherein said analog comprises
  one or more naturally occurring amino acids, non-naturally occurring amino acids, modified
  amino acids, or amino acid mimetics.
- 3. The HLA-binding peptide inhibitor of Claim 2, wherein said analog is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.
- 4. The HLA-binding peptide inhibitor of Claim 1, wherein said immunogenic gluten oligopeptides comprises at least one PXP motif.
- 5. The HLA-binding peptide inhibitor of Claim 1, wherein said immunogenic gluten oligopeptides comprises a sequence selected from the group consisting of: PQPELPY; PFPQPELPYP, PQPELPYPQPQLP, PQQSFPEQQPP, VQGQGIIQPEQPAQ, FPEQPQQPYPQQP, FPQQPEQPYPQQP, FSQPEQEFPQPQ; PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PYPQPELPY and PYPQPQLPY.
- [96] 6. The HLA-binding peptide inhibitor of Claim 1, wherein said inhibitor comprises the sequence PXPQPELPY, where X is Tyr, Trp, Arg, Lys, p-iodo-Phe, 3-iodo-Tyr, p-amino-Phe, 3-amino-Tyr, hydroxylysine, ornithine, Asp or Glu.
  - 7. The HLA-binding peptide inhibitor of Claim 6, wherein said inhibitor is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.
  - 8. The HLA-binding peptide inhibitor of Claim 6, wherein said inhibitor is further modified to increase binding potency to an MHC molecule.
  - 9. The HLA-binding peptide inhibitor of Claim 1, wherein said inhibitor comprises the sequence  $PFPQX_1ELX_2Y$ , where  $X_1$  and  $X_2$  are independently selected from 4-hydroxy-Pro, 4-amino-Pro, or 3-hydroxy-Pro, and proline, with the proviso that at least one of  $X_1$  and  $X_2$  is a residue other than proline

10. The HLA-binding peptide inhibitor of Claim 9, wherein said inhibitor is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.

- 11. The HLA-binding peptide inhibitor of Claim 9, wherein said inhibitor is further modified to increase binding potency to an MHC molecule.
- 12. A method of treating Celiac Sprue and/or dermatitis herpetiformis, the method comprising:

administering to a patient an effective dose of an HLA-binding peptide inhibitor; wherein said HLA-binding peptide inhibitor attenuates gluten toxicity in said patient.

- 13. The method of Claim 12, wherein said HLA-binding peptide inhibitor is administered with a glutenase.
- 14. The method according to Claim 12, wherein said HLA-binding peptide inhibitor is administered orally.
- 15. The method according to Claim 12, wherein said HLA-binding peptide inhibitor is contained in a formulation that comprises an enteric coating.
- 16. A formulation for use in treatment of Celiac Sprue and/or dermatitis herpetiformis, comprising:

an effective dose of an HLA-binding peptide inhibitor and a pharmaceutically acceptable excipient.

- 17. The formulation according to Claim 16, further comprising an enteric coating.
- 18. Use of an HLA-binding peptide inhibitor in the treatment of HLA-DQ2 positive individuals who are either pre-disposed to type I diabetes or have developed symptoms of type I diabetes.
- 19. A computer for producing a three-dimensional representation of a molecule wherein said molecule comprises an HLA-DQ2 molecule bound to an immunogenic gluten oligopeptide, wherein said computer comprises:
- a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the three-dimensional coordinates of a subset of the atoms in an HLA-DQ2 molecule bound to an immunogenic

gluten oligopeptide;

a working memory for storing instructions for processing said machine-readable data;

- a central-processing unit coupled to said working memory and to said machinereadable data storage medium for processing said machine readable data into said threedimensional representation; and
- a display coupled to said central-processing unit for displaying said three-dimensional representation.
- 20. A computer-assisted method for identifying potential modulators of Celiac Sprue and/or dermatitis herpetiformis, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
- (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in an HLA-DQ2 molecule bound to an immunogenic gluten oligopeptide, thereby generating a criteria data set;
- (b) comparing, using said processor, said criteria data set to a computer database of chemical structures stored in said computer data storage system;
- (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said criteria data set;
- (d) outputting to said output device the selected chemical structures having a portion similar to said criteria data set.